

विज्ञान एवं प्रौद्योगिकी विभाग DEPARTMENT OF SCIENCE & TECHNOLOGY

Research & Technology Development Compendium on **MATERIAL FOR ENERGY STORAGE** (Clean Energy Research Initiative)





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Dr. Ranjith Krishna Pai received the Ph.D. degree in Natural Sciences, from Dr.Othmar Marti's Group, Ulm University, Germany, in 2005. He is currently Scientist 'E' / Director of Technology Mission Division of Department of Science and Technology responsible for research, development and innovation activities in Clean Energy domain. He has represented India in numerous multi lateral event and has articulated national and international endeavors in energy domains.

From 2006 to 2007, he was a Postdoctoral Researcher at University of Chile, Santiago, aworking on Genetic engineering of a novel protein-nanoparticle hybrid system with great potential for bio sensing applications. 2007 to 2009, he spent two years as a Post-Doctoral Scientist at Stockholm University, Stockholm, Sweden, working on synthesis of nanostructured hybrid materials and Characterization of nonlinear optical nanomaterial. From 2009 to 2011, he was a Research Scientist at CFN, Brookhaven National Laboratory, New York, USA, working on photo fabrication of donor- acceptor antenna system for solar energy harvesting, development of bio sensing platforms based on bio-inorganic scaffolds with single molecule/particle sensitivity, fabrication of transparent organic thin-film for use in organic photovoltaic cells. After spending 2 years 5 months at BNL, New York, USA, he spent another 2 years 4 months (2011-2013) as a Research Scientist at INL - International Iberian Nanotechnology Laboratory, Braga, Portugal. His research at INL involved development of transparent conjugated polymer films for capturing solar energy, organic thin-film solar cells based on conjugated polymers and fullerene derivative, hybrid organic/inorganic nanomaterial and synthesis and fundamental study of conjugated polymers, solar device fabrication and electrical and photochemical device measurements.From 2013 to 2015, he was an Associate Professor and Group leader at Nanostructured Hybrid Functional Materials & Devices, Jain University, Bangalore, India.

He published several high impact scientific papers, and author of three book chapters.15 invited lectures at international conferences. Previously served as an Associate Editor of a Journal "Nano tools & Nano machines" and a Guest Editor of International Journal of Polymer Science. His research interest includes energy conversion technologies, including low cost photovoltaic (Organic, and hybrid solar cells) and electrical energy storage (batteries and supercapacitors), synthesis of semiconducting polymers and polymer nanostructures and their application to organic transistors, solar cells, light emitting diodes and other photonic applications, synthesis, characterizations and applications of carbon and inorganic nanotubes, Modeling of the electronic properties of nanostructured semiconductors.



#### Dr. Rajiv K. Tayal

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Dr Rajiv Tayal has been working as an Advisor in the Department of Science & Technology (DST), and is currently heading the Technology Mission Division which is concerned with major R&D initiatives in the areas of Clean Energy and Water, including international programs with several other countries.

He presided over two of the most prestigious institutions in the Indian S&T ecosystem in the immediate past; as Executive Director of the bi-national Indo-US Science & Technology Forum (IUSSTF) and Secretary of the Science & Engineering Research Board (SERB).

His extensive professional experience in Science, Technology and Innovation space, spans across Industry, Government and a large number of academic institutions, research laboratories and industry. He is a Fellow of the Indian National Academy of Engineering, FNAE and The Institution of Engineers (India), FIE.

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<u>Message</u>

27.04.2021

Materials discovery and development crosscut the entire energy technology portfolio, from energy generation and storage to delivery and end use. Materials are the foundation of every clean energy innovation: advanced batteries, solar cells, lowenergy semiconductors, thermal storage, coatings, and catalysts for the conversion, capture, and use of carbon dioxide. In short, new materials constitute one of the cornerstones for the global transition to a low-carbon future. The process of discovering and developing new materials currently entails considerable time, effort, and expense. Each newly discovered molecule is run through simulation, synthesis, and characterization, with synthetic procedures taking from 10 to 20 years at a very high cost. Materials discovery and development, however, are at the cusp of a transformational change that could reduce the time to design, optimize, and discover new materials by at least 10 times, cutting it down to one or two years. Recognizing the challenges and opportunities associated with materials discovery, Department of Science & Technology under its Clean Energy Research Initiative (CERI) mounted a thematic research and technology programme on energy materials. Materials for Energy Storage (MES) has supported novel energy storage research proposals to identify the most promising breakthrough opportunities for accelerating the materials discovery process. The initiative also anticipated research on the different aspects of the overall system, such as development of computational materials with next generation computing artificial intelligence (machine learning) and robotic tools, new materials & devices including scale-up and cost, application & integration of material into devices with the aim of creating a more fully integrated approach. The report presents portfolio of R&D projects taken up in this initiative with the participation of several scientists, industries, utilities and other stakeholders from R&D laboratories, academia and industries related to Clean Energy. I hope that this compendium will enable researchers and stakeholders connect and collectively contribute to Clean Energy research, development, demonstration and deployment.

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(Ashutosh Sharma)

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## INTRODUCTION

The Department of Science and Technology, as part of its Clean Energy Material Initiative, Materials for Energy Storage (MES) was launched in 2016 to support Material for "Energy storage research including breakthrough research for materials leading to disruptive innovations in energy storage and may address all areas of energy storage technologies including: Chemical and electrochemical technologies (including alternatives to critical metals used in efficient energy storage); Electrical technologies; Mechanical and thermal storage technologies. The research primarily addresses stationary applications and distribution of electricity. Research may range from the development of improved storage systems for electricity grids to the demonstration and assessment of new technologies and systems analysis issues.

MES 2018 has received a total of 228 proposals against the call out of which 26 projects have been supported.

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### High Performance Aqueous Redox Flow Batteries Based On Redox Active Polymers And Janus Membranes

#### **Background of the Project**

The need of the hour is to create a large-scale energy storage system to integrate renewable energy sources, such as solar and wind, to be effectively used in the grid and to avoid the output fluctuation. Redox Flow Batteries (RFBs) has received tremendous attention for this kind of energy storage. Vanadium-based RFBs received much attention; however, its low volumetric energy storage capacity, the limite solubility, and need of ion exchange membranes are some of the major drawbacks. Recently, redox organic polymers have been proposed as charge-storage materials, which are potentially low-cost, soluble in a range of solvents, along with the possibility to tune their redox properties, solubility, and crossover by introducing different substituents. Recent developments towards developing water-soluble redox active polymeric materials have opened a new avenue for developing more safer and greener RFBs. However, water-soluble polymers and membranes with very high selectivity are crucial for this kind of RFBs. Here, we are targetting to synthesize ne polymers with enhanced solubility and redox activity along with fabrication of novel Janus membranes for better selectivity and low crossover of active polymers.

#### Aim

The project is intended to develop a novel aqueous Organic Polymer based Redox Flow Battery (ORFB) system based on Janus nanoporous and charged membranes as well as tailor-made electro/redox active organic oligomers and polymers. We are aiming to develop two crucial components, i.e., Janus membrane separator and redox active polymers for aqueous organic polymer based ORFB system.

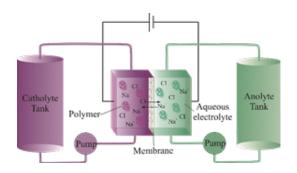
#### **Methodology**

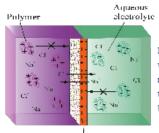
To realize the full potential of ORFB, we are developing novel tailor-made redox-active polymers and Janus membranes, which are critical components for this type of battery. Our focus is water-soluble redox-active polymers based on monomers with redox-active moieties and Janus membranes to achieve high cell performance by limiting the crossover of materials and long-term application. The functionalization of these polymers is also be undertaken by introducing aqueous solubilizing units such as cationic and anionic functional groups. The second part of the work plan is to fabricate charged and ion conductive nanoporous Janus membranes by chemical modification or layer by layer deposition method with well-defined nanopores to control the ionic transport as well as selectivity with respect to anolyte and catholyte. We are analysing the Janus membranes regarding molecular weight cut-off (monomer to oligomer and polymer), surface charges, ion conductivity, diffusion and crossover, and their electrochemical behaviour. Finally, we have fabricated a lab-scale prototype RFB consist of Teflon support and flow chambers, current collectors, EPDM gaskets, graphite felt electrodes and reservoirs for catholyte and anolyte connected to a peristaltic pump. We are assessing the galvanostatic charging/discharging of the developed batteries and their life cycle assessment.

#### **Expected Outcome & Deliverables**

Novel water soluble redox-active polymers with unexceptional electrochemical properties.

- Highly selective nanoporous Janus membranes with excellent size exclusion based on size and charge nature of the redox active polymers.
- A lab scale prototype organic polymer based redox-flow battery using synthesized polymers and Janus membranes.
- Characterization and performance assessment of ORFB under neutral pH and aqueous condition.
- Publications in high impact journals, patent, and dissemination of results in conferences and symposia.
- Training of young researchers towards PhD degree.
- Although the proposed ORFBs will be green, with longer lifetime, and performance, its cost depends upon the polymers and membranes. We believe that it will be competitive with traditional rare earth metal based RFBs.



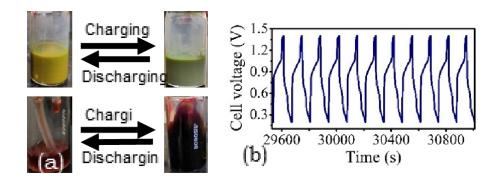


Janus membrane (Charge affinity barrier)

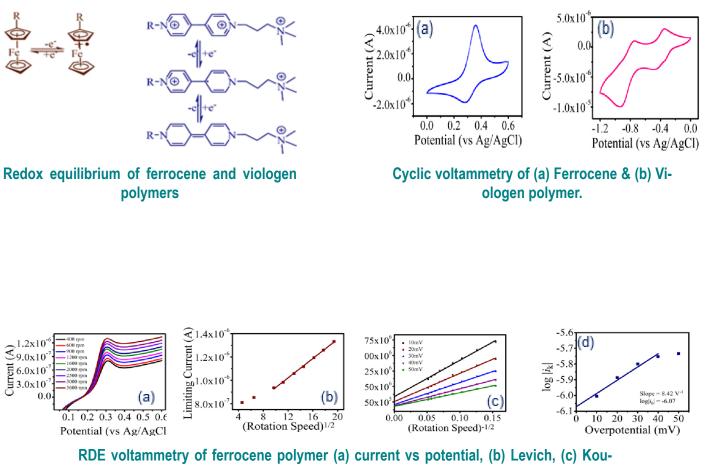
Demonstration of electrochemical cell with a Janus membrane. The membrane allows only the small ions to pass, while rejects active materials by creating a charge affinity barrier



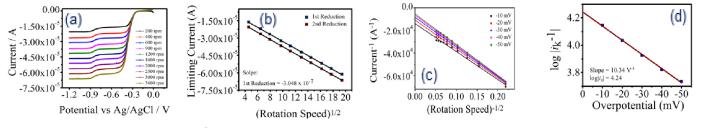
ORFB prototype developed at DMSE, IIT Delhi



(a) Colour change of catholyte and anolyte polymers (b) Charge/discharge curves.



tecky-Levich, & (d) Tafel plot.



RDE voltammetry of viologen polymer (a) current vs potential, (b) Levich, (c) Koutecky-Levich, & (d) Tafel plot.



#### Dr. Bijay P. Tripathi Assistant Professor, IIT Delhi, New Delhi Email: bptripathi@iitd.ac.in

Prof. Tripathi received his Masters in Organic Chemistry from DDU Gorakhpur University in 2006 and Ph.D. from CSIR-CSMCRI, Bhavnagar, in 2011. He was an Alexander von Humboldt postdoctoral fellow from 2011-13 in the group of Prof. M. Stamm at the Leibniz Institute of Polymer Research Dresden, Germany, where subsequently undertook Group Leader position prior to starting his independent career as an Assistant Professor at the Department of Materials Science & Engineering, IIT Delhi. During his research career, he has been awarded with prestigious fellowships such as DAAD and Humboldt fellowship (Germany), JSPS (Japan), Marie-Curie Fellowship (Eur. Comm.), DST-INSPIRE and UGC-FRP. Prof. Tripathi's research spreads around polymer and nanomaterials synthesis, surface functionalization, nanoporous and charged membranes, and nanocomposites for applications ranging from energy, water, separation, catalysis, & environmental remediation. His research group's interest is targeted towards redox polymers for aqueous redox flow battery, materials for energy storage and heat management, self-cleaning surfaces, COFs and MOFs, and artificial cells for biosynthesis.

## **Oxynitride-Composites Base Low Weight** Supercapacitor Unit: Materials Enhancement And Device Developments

#### Aim

We propose to develop a low cost supercapacitor device, enclosed in a plastic containment, using entirely indigenously developed materials, at IIT Madras. The system will be based on advanced nanostructured oxynitride based materials to enable Faradaic and hybrid supercapacitors. Furthermore a plastic containment will be used to package the supercapacitors. Scaling up using a series/parallel combination of capacitors will also be explored, at the latter stages of this project. IITM's Climate chamber will be used for field trials, in efforts to enhance the Technology Readiness Level of the deliverable to 3-4 at least.

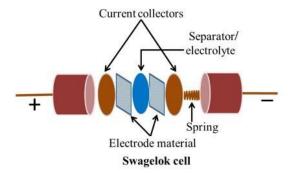
#### Methodology

- Novel oxynitride based nanocomposites will be developed and tested.
- The usual oxynitride bottleneck associated specific surface area will be overcome using novel synthetic approaches; the capability for which is there in the group.
- All essential materials and electrochemical characterization techniques will be used to study the material, and its performance on device deployment..
- Unique and essential combination of chemical and engineering approaches is used here, to achieve a technology oriented deliverable.
- IITM's Climate chamber will be used for field trials, in efforts to enhance the Technology Readiness Level of the deliverable to 3-4 at least.

#### **Expected Outcome & Deliverables**

- Specific capacitance of ~few thousands F g-1 using (potentially green) oxynitride materials and related composites will be achieved.
- Series resistance will be minimized and brought down to <10 milliohm; shunt resistance will be brought up to a few mohms.
- Optimization of several parameters such as current collectors and electrolytes
- IITM's Climate chamber will be used for field trials, in efforts to enhance the Technology Readiness Level of the deliverable to 3-4 at least. This takes would ensure that the deliverable is roughly at Technology Readiness Level 3-4 (on a 10 point scale).





Swagelok cell solid state capacitor for testing in climate chamber and its flow diagram. Here electrode material is oxynitride based material.

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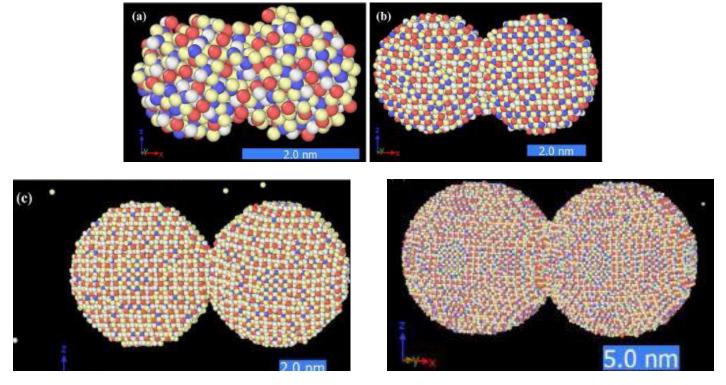


Figure 1. a–d The interaction of particles of various diameters 2, 4, 6 and 10 nm at 1400 °C, respectively. It can be seen that above the ~ 6-nm size regime, Ba, O, and N escape from the surface. Red, blue, yellow and white spheres represent Ba, Ta, O, and N, respectively



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Dr. Tiju Thomas received his MS and PhD degrees from School of Engineering at Cornel University, Ithaca, NY, USA. Prior to his doctoral studies at Cornell, he acquired masters (M.S (Engg.)) at the Theoretical Sciences Unit in Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore. He was also working on an industry - academia joint project involving University of Toronto, Memorial University of Newfoundland, and Lumentra Inc. (astart-up company, specializing in light emitting devices). Then he moved to India as a Faculty Fellow at the Materials Research Center in the Indian Institute of Science (IISC), Bangalore. After two years of working at IISC Bangalore, he joined the Department of Metallurgical and Materials Engineering (Indian Institute of Technology Madras, IITM) in Chennai. Currently he Associate Professor and Head of Applied Nanostructures Engineering and Nanochemistry (ANEN) research group. His research focuses is on developing compositionally complex oxides, oxynitrides and nitrides, and nanometals for achieving engineering ends. Problems concerning functional properties of materials (electrical and electronic, optical, magnetic; applied surfaces and interfaces).

## **B** Vertically Oriented Graphene Nanosheets On Graphite For High Specific Capacity Ultracapacitor Electrode

#### Aim

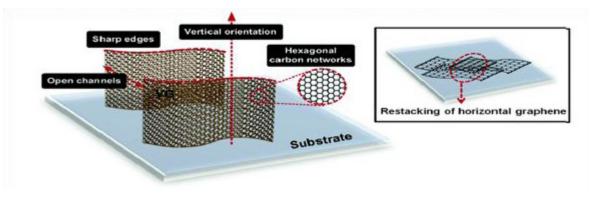
The project aims at developing an ultracapacitor electrode with a specific areal capacitance of more than 2.5 F/cm<sup>2</sup> and 125 F/g, both @ 1mA/cm<sup>2</sup>. The synthesized electrode will be used to fabricate a symmetric capacitor of energy density more than 10 Wh/kg.

#### Methodology

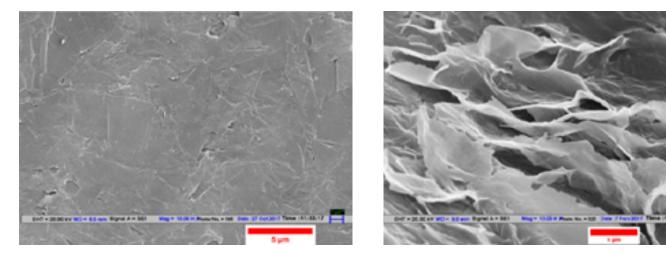
Vertically Oriented Graphene Nanosheets (VOGN) will be one of the targeted morphologies for the electrode. Electrochemical treatment of graphite, including partial exfoliation will be used for the synthesis of the electrode. Sulfuric acid is selected as the electrolyte for exfoliation and a systematic study will be undertaken to understand the effects of synthesis conditions (i.e. Sulfuric acid concentration, electrode potential, exfoliation current density, time of exfoliation and pre- treatment) on the density, stability and number of layers of VOGN on graphite.

#### **Expected Outcome & Deliverables**

• Graphite supercapacitor based electrode of areal capacitance for of 2.5 F/ cm<sup>2</sup> @ 1mA/cm<sup>2</sup> which is about 2-times the best value reported for VOGN electrodes. The initial studies will be done with graphite electrode size of 1 cm<sup>2</sup> (~0.01g) and later will be scaled up to 25 cm<sup>2</sup> (0.25 g).



Vertically oriented graphene nanosheets on a substrate. The inset shows the orientation when nanosheets stack together and orient parallel to the substrate.



SEM images of HOPG and a partially exfoliated HOPG covered with VOGN



**VOGN** based ultracapavitior



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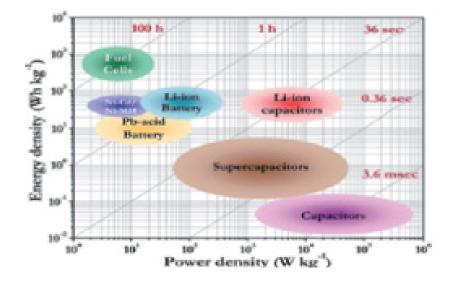
Professor Anupam Shukla received his Ph.D. from IIT Kanpur in 2004. He has been associated with several industrial and research projects sponsored by ONGC, CSIR, DST, FIIT and SERB. His current research is focused on supercapacitive energy storage, structural characterisation of graphite intercalated compounds, graphene synthesis by electrochemical exfoliation and electrochemical oxidation of aqueous sulfur dioxide.

**Compendium on MES 2018** 



#### Aim

Development of prototype lithium ion capcitor with high energy density by internally hybridizing a super capacitor electrode and lithium ion battery electrode. Ragone plot showing the energy density and power density of different energy storage devices



#### Methodology

The research project involves the synthesis of carbon aerogel suitable for lithium ion capacitor positive electrode application through super critical drying method. The novel concept of using composite positive electrode containing sacrificial salt for safe prelithiation will be explored. Prototype lithium ion capacitor will be developed using graphite/carbon aerogel electrodes system and their electrochemical performance will be studied.

#### **Applications**

Lithium ion capcitor can be used in mobile applications such as energy recuperation in cars, buses, Light Rail Vehicles (LRV), trams and other commercial vehicles. They also contribute to performance improvement of stationary systems such as backup storage, peak assist, power quality, electricity storage etc.

#### **Expected Outcome & Deliverables**

- Carbon aerogel with optimum properties suitable for application in lithium ion capacitor
- Easy methodology for prelithiation of lithium on capacitor
- Advanced hybrid Electrochemical energy storage system with graphite/car bon aerogel electrodes having higher energy density than conventional super capacitor and comparatively higher power density than lithium ion battery



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Dr Stanly Jacob K. received M.Sc Chemistry Degree from Bharathidasan University and Ph.D from Calicut University. His current research interest includes Lithium ion capacitor, low cost electrode materials for super capacitor, hybrid super capacitor, application of inorganic and organic aerogel for energy applications.



### Fabrication And Demonstration Of All-Solid-State High Performance Flexible Supercapacitor Device

#### Aim

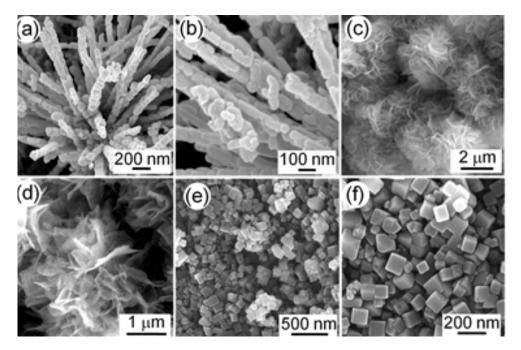
Design and development of highly efficient hybrid materials involving metal oxides/ chalcogenides and carbon supports ( $g-C_3N_4$ , N-doped graphene hydrogel, and /or conducting polymers) as active materials for all-solid-state supercapacitors using polymeric membrane and/or gels as separator. To increase the energy density of the fabricated two-electrode (symmetric or asymmetric) devices with life-cycles more than 10000 cycles without deteriorating performance below 90%.

#### **Methodology**

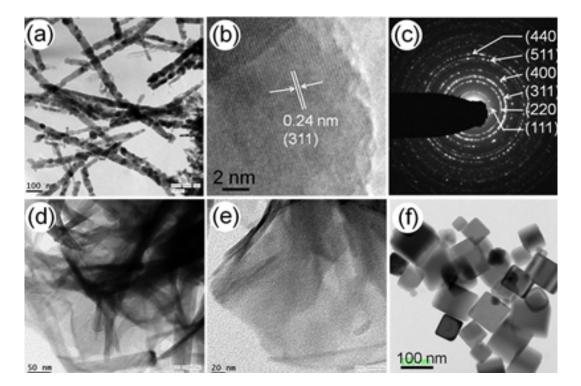
The importance of present work lies in designing and synthesizing porous high surface-area nanostructured oxides and chalcogenides using solution based techniques (microwave hydrothermal/ solvothermal) in a short duration (less than 30 min). Synthesizing hybrid materials using appropriate conducting carbon/ polymer support. After optimizing the energy storage performance of the synthesized materials, both asymmetric and symmetric device will be fabricated by coating the active materials on the conducting support. The performance will be demonstrated by running portable electronic devices such as light emitting diodes etc.

#### **Expected Outcome & Deliverables**

 Several nanostructured materials with controlled shapes and sizes will be delivered in this work. Those materials will not only have potential supercapacitor but also in other applications. Novel in polymeric membranes that can be used as separator for the supercapacitor device.



FESEM images of the Co3O4 nanostructured materials with different shapes and sizes synthesized in our laboratory using microwave solvothermal technique.



Transmission electron microscope images of the Co3O4 nanostructured materials with different morphologies.



## Photographs on powering small devices using the fabricated Co3O4//graphene hydrogel asymmetric supercapacitor device.



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Dr. Debabrata Pradhan has received Ph.D. degree from IIT, Bombay, under the guidance of Prof. Maheshwar Sharon in 2003. In Ph.D., he worked on the synthesis of carbon nanomaterials (nanotubes and fibers) from camphor and kerosene. After completing Ph.D. work, he served the Electron Microscopy lab of Sophisticated Analytical Instruments Facility (SAIF) at IIT Bombay for a year before moving to Taiwan in 2004 for the postdoctoral research. In Taiwan, Dr. Pradhan worked on ultrananocrystalline diamond thin films by microwave plasma deposition and their application in electron field emission. In 2006, he moved to Canada and worked at University of Waterloo for four years. In this period, he extensively worked on electrodeposition of several oxide nanomaterials and their application in glucose sensor, electron field emission, and hydrogen generation. His present research focuses on the synthesis of nanostructured materials for the renewable energy generation and storage. The synthesized materials by his group are primarily used for water-splitting reaction, alcohol fuel cells, and perovskite solar cell as energy conversion systems and supercapacitors for energy storage. Dr. Pradhan has more than 120 international referred journal publications, 2 Indian patents, 1 book, and 2 book chapters to his credit. His present h-index is 37 (Google scholar).

# 6

## **2D Material Informatics for Lithium ion Storage**

#### Aim

Aim: We propose to deliver 2D material portfolio for next-generation Li-ion battery anode. Novelty of our proposal lies in its approach, which is combination of fundamental-science-driven (high-throughput first-principles based calculations and experiments) and data-driven (machine learning).

#### Methodology

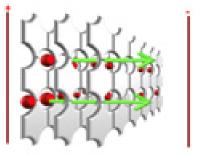
- Use of cutting-edge processor technology (accelerators) to implement "High-Throughput Density Functional Theory (HT-DFT)" calculation.
- Use of new 'linearly-scaled' 'finite-temperature' DFT code for modeling very large atomic structure.
- Focus is on 2D materials, which promise superior Lithium ion storage due to inherit large volume to mass ratio.
- Machine learning techniques to create 2D material database for Lithium ion battery anode. Use of crystal orbital Hamiltonian as one of the signatures for machine learning.
- Use of novel wet chemical design methods like solid state, sol-gel, colloidal synthesis as well as physical methods e.g. scotch-tape exfoliation, liquid exfoliation and chemical vapor deposition will be employed to obtain few layered 2D TMDs.

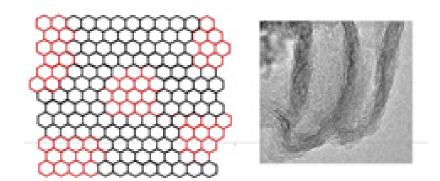
 For experimental verification of the theoretical findings, State of the art structural and electrochemical characterization including in situ spectroscopic and diffraction methods using Institute and synchrotron facilities at DESY, Hamburg and Elettra, Trieste.

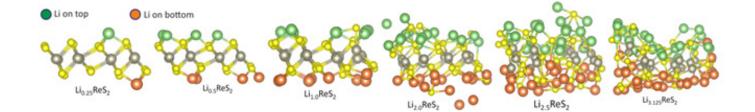
#### **Expected Outcome & Deliverables**

- 2D material database for Lithium ion battery anode with their specific capacity and diffusion co-efficient.
- Computer program for machine learning algorithm.
- Recipe for high-throughput ab-initio calculations in hybrid processor (CPU GPU) based supercomputers.
- Assembly of batteries with select 2D materials (with/without carbon additives) having optimized structure and properties.











#### Dr. Santanu Mahapatra Professor Indian Institute of Science, Bangalore

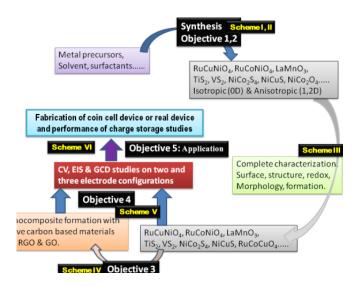
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Received his B.E. (Bachelor of Engineering) degree from Jadavpur University, Kolkata, in the field of Electronics and Telecommunication in 1999, M. Tech (Master of Technology) degree in the field of Electrical Engineering (specializing in Microelectronics) in 2001 from Indian Institute of Technology (IIT) Kanpur, and Ph.D. degree from Swiss Federal Institute of Technology Lausanne (EPFL) in 2005. For his Ph.D. dissertation he worked on the modeling of Single Electron Transistor (SET) and its co-simulation and co-design with CMOS. He joined Department of Electronic Systems Engineering (formerly CEDT), at Indian Institute of Science (IISc), Bangalore, India, as an assistant professor in August 2005 and promoted to associate professor and then full professor rank in September 2010 and December 2015 respectively. He founded Nano Scale Device Research Laboratory in 2006, where his research team engaged in modeling of carrier transports in nano materials at circuit, device and atomistic level. His research interests include two dimensional channel transistors, energy efficient electronic switches and energy-storage at nano-scale. He is the author of the book Hybrid CMOS Single Electron Transistor Device and Circuit Design. He received IBM Faculty award in 2007, Microsoft Research India Outstanding Faculty Award in 2007 and the associateship of Indian Academy of Sciences in 2009. He is also the recipient of Ramanna Fellowship (2012 to 2015) in the discipline of electrical sciences from Department of Science and Technology, Government of India for his contribution in compact modeling. He is senior member of IEEE and Associate Editor of Sadhana.

## Development Of Nanostructured Mixed Metal Oxide And Metal Chalcogenide Materials Based Effective Electrodes And Their Use In Super capacitor Devices

#### Aim

Synthesis & characterization of novel morphology oriented Mixed Metal Oxide (MMO) nanoparticles suitable for charge storage devices. Synthesis & characterization of novel morphology oriented Metal Chalcogenide (MC) nanoparticles suitable for charge storage devices. Preparation of nanocomposites of MMO & MC nanoparticles with active carbon materials (RGO) and characterization. Making of electrodes and studies on charge storage characteristics by CV, EIS & GCD on three electrode configuration. Fabrication of devices (flexible or coin cell) and performance of charge storage studies.



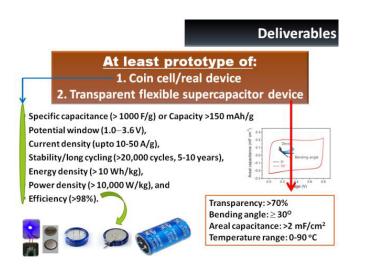
#### **Methodology**

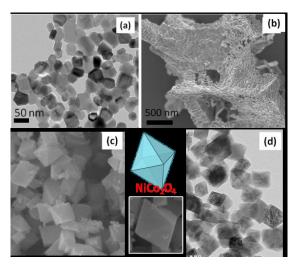
Novel materials with novel combination of mixed valence metal ions, varied shape and high porosity from novel synthesis methods. Innovative synthesis of isotropic/ anisotropic mixed metal oxide nanoparticles.

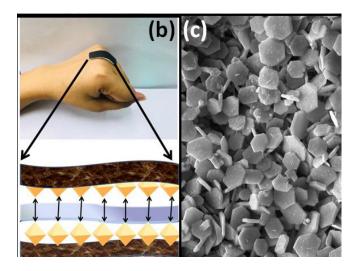
- 1. Innovative synthesis of isotropic/anisotropic metal chalcogenide nanoparticles.
- 2. Studies on the structural, surface, morphology and redox properties.
- 3. Preparation of nanocomposites from MMO and MC with RGO.
- 4. Making of 3 electrode configuration and studies on charge storage characteristics by CV, EIS & GCD.
- 5. Fabrication of coin cell device or real device and performance of charge storage studies.

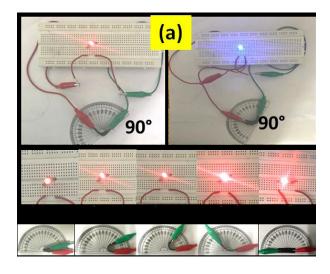
#### **Expected Outcome & Deliverables**

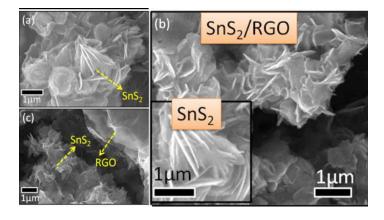
This proposal will deliver a few best supercapacitor devices from low cost environmental friendly very efficient electrode materials, where the target performance would be: specific capacitance (> 1000F/g), potential window (1.0-3.6 V), current density (upto 50 A/g), stability/long cycling (>20,000 cycles, 5-10 years), power density (> 10 Wh/kg), energy density (> 10,000 W/kg), and efficiency (>90%). These targets are expected to be better than national & international products at much cheaper cost.

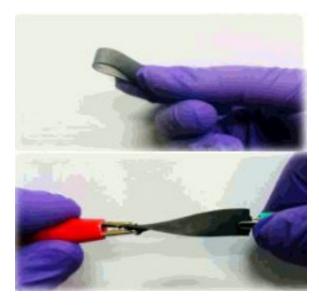














#### Dr. Sasanka Deka Associate Professor University of Delhi, North Campus, Delhi Email: sdeka@chemistry.du.ac.in

Dr. Sasanka Deka received his M.Sc. in Chemistry from Gauhati University, Guwahati in 2001 and Ph.D. degree from National Chemical Laboratory (NCL-Pune) in 2007. He has been awarded the TMS Foundation 2008 Shri Ram Arora Award, by the TMS, Warrendale, USA for his contribution to materials science. He then moved to National Nanotechnology Laboratory, CNR-INFM, Lecce, Italy and Italian Institute of Technology, Genova, Italy for postdoctoral research in the nanochemistry. Dr. Deka has published more than 55 research papers in different international peer-reviewed journals and meetings, and also wrote 2 books and 1 book chapter published by international publisher. He has been awarded with DAE-BRNS Young scientist research award; Visiting Fellow, School of Physical Sciences (SPS)-JNU; VIFA-Chennai outstanding faculty (Chemistry) award 2019; Adjunct Faculty (2017): Chemistry, Islamic University of Science & Technology (IUST), Jammu and Kashmir. His current research interest deals with synthetic nanochemistry, multifunctional hybrid nanocrystals, novel nanostructured materials for energy research.

# 8

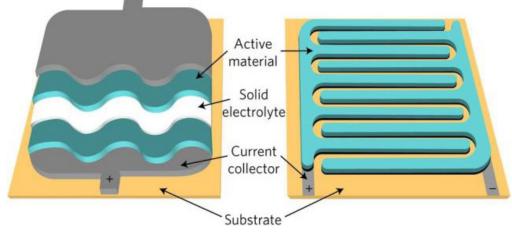
## Fabrication Of High Energy Density Thin Film Based On-Chip Supercapacitor Devices Using Reactive Magnetron Sputtering

#### Aim

The prime objective of this project is to develop on-chip supercapacitors operating in a wide temperature range with improved electrochemical performance by exploring novel electrode materials. Fabrication and performance study of onchip supercapacitor device which could be used directly for micro-electronics industry after scaling.

#### Methodology

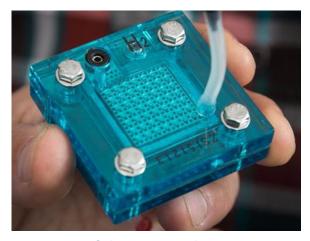
Complete electrode preparation would be performed in a single step using DC Reactive Magnetron Co-sputtering technique. The various sputtering parameters such as working pressure, base pressure, substrate temperature, gas flow ratio and DC/RF power will be initially optimized separately to fabricate high quality hybrid thin films. The structural and complete electrochemical characterization of the three electrode system and the devices would be performed.



Microsupercapacitor components

#### **Expected Outcome & Deliverables**

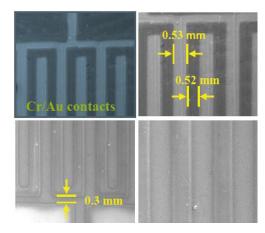
- Fabricated electrodes with large area.
- Deposition without any binder and any other external treatment.
- Prototype device based on fabricated
- supercapacitor electrodes.
- Intellectual property right, if any.



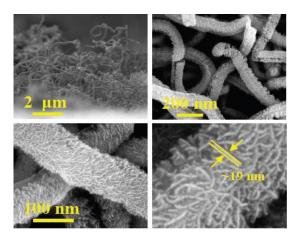
Solar supercapacitor



PMP9766 Supercapacitor Backup Power Supply

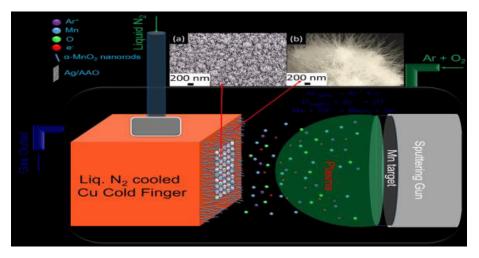


**On-chip supercapacitor** 



MoS2-CNT hybrid supercapacitor

Compendium on MES 2018



Thin film electrode Fabrication



#### Dr. R. Chandra Assistant Professor Indian Institute of Technology, Roorkee Email:ramesfic@iitr.ac.in

Prof R. Chandra received his Ph.D. in Experimental Condensed Matter Physics from Indian Institute of Technology Delhi in 1993. He has worked as a visiting scientist at Tata Institute of Fundamental Research Mumbai, India (1997-99), and University of Cambridge, UK (2003-04). He has completed several research projects sponsored by various agencies of Govt. of India such as DST, CSIR, DRDO, DAE, CPRI and several are under process. He has supervised 25 Ph.D. students and currently supervising 8 students in diverse areas of Nanoscience and nanotechnology. His current research is focused on the development of nanostructured thin films by PVD for gas sensors and energy storage applications.

## High-Performance Graphene-Based Supercapacitors

## Aim

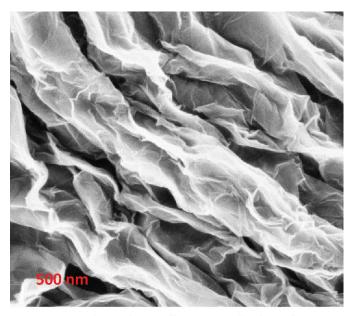
We propose an unconventional approach of producing Reduced Graphene Oxide (RGO) which can be readily used as an active material for the fabrication of supercapacitor electrodes. The reducing agent can be re-generated for the subsequent feeds of the reduction of Graphene-Oxide (GO). Additionally, we plan to unveil the importance of the composition of greener Gel Polymer Electrolyte (GPE) systems than often flammable and eco-unfriendly organic electrolytes as well as ionic liquids in RGO supercapacitor applications. Since in our chemical reduction we can prepare semiconducting RGO, we plan to use distinctively doped RGO material in tuning the performance of supercapacitor.

## **Methodology**

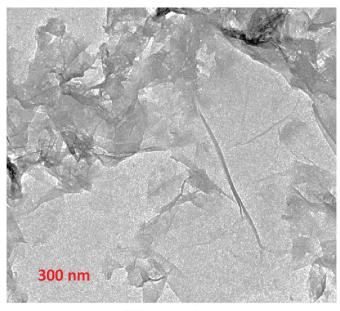
The focus of the proposed research plan encompasses simple synthesis involving oxidation and reduction with the usage of transition metal salts as reducing agents (PI's own Indian Patent Application No. 201621023063; status published). This is further associated with quality assurance in batch production of RGO, state-of-art characterization of RGO, tuning of GPE composition and evaluation of electrochemical performance in lab followed by prototype device testing at SPEL Pune.

## **Expected Outcome & Deliverables**

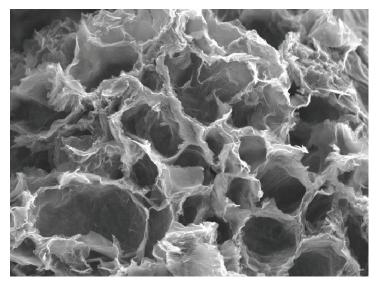
- Development of relatively low-cost porous rGO with 2D and 3D morphological patterns along with an emphasis on greener GPE
- 50 gm rGO per year
- Supercapacitors of capacitance of 10 F (10 numbers) and 500 F (10 numbers) with energy density of 20 Wh/kg
- The focus will be on the building-up of a strong academy-industry interface (IISER Pune Surya Powerfarad Energies Ltd. (SPEL) Pune)



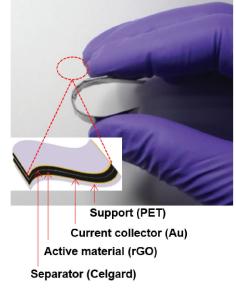
reduced graphene oxide (rGO)



rGO nanosheets



3D mesoporous rGO



All-solid-state flexible rGO supercapacitor



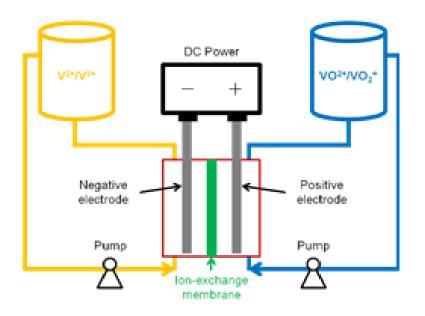
Dr. Nirmalya Ballav Assistant Professor Indian Institute of Science Education and Research, Pune E-mail: nballav@iiserpune.ac.in

Dr. Nirmalya Ballav has completed his M.Sc. in Organic Chemistry (2000) and Ph.D. in Physical Chemistry from University of Calcutta, India (2005). Before joining IISER Pune as an Assistant Professor in 2011, he was postdoctoral fellow at Applied Physical Chemistry, University of Heidelberg, Germany and at Laboratory for Micro and Nanotechnology, Paul Scherrer Institute (PSI, ETH Domain), Switzerland. He is a Visiting Scientist at PSI since 2011. His primary research focuses on interfacial materials chemistry (from fundamentals to applications) – exploring various solid-sloid and solid-liquid interfaces and capturing interesting interfacial effects. Research platforms include two-dimensional materials, coordination polymers, conducting polymers, metal nanoparticles, and magnetic semiconductors. He has published over 100 research papers in international journals with hi-index of 34.

## **10** Design, Development And Demonstration Of 1 Kw (1 Kwh) Vanadium Redox Flow Battery For Stationary Application

## Aim

Development of an efficient 1 kW (1 kWh) vanadium redox flow battery using low cost membrane and efficient electrode. Development of battery management system for VRFB along with integration and packaging of Vanadium Redox Flow Battery (VRFB) and its demonstration.



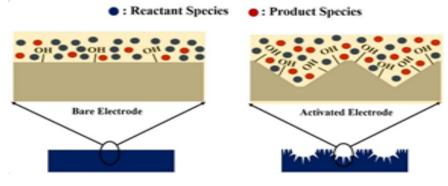
(Typical Vanadium redox flow battery; Open Source)

## Methodology

It research work is primarily applied in nature. The following methodology will be used,

- Surface oxygen functional groups on the carbon electrode acts as active sites and thus functionalization of electrode will be done by a novel chemical activation method. The preliminary analysis shows an improvement of ~150% in the charge
- transfer reaction without the use of any electrocatalyst.

- Pore-filling membrane will be used for the VRFB membrane cum separator. These
  membrane would be inexpensive as compared to nafin membrane and will reduce
  the vanadium crossover. Further, evaluation of doped nafion with SiO<sub>2</sub> or TiO<sub>2</sub> will
  also be carried out.
- Conventional BMS is not suitable for the flow battery. Therefore, BMS will be designed or retrofitted with the help of the Industrial and academic partners.



(Typical surface structure of electrode)

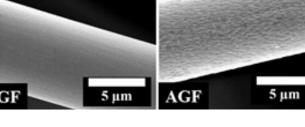
### **Expected Outcome & Deliverables**

 Full VRFB system will be developed and demonstrated with the following achievable specifications (in-line with the IREDA requirement for home light systems).

•	Current density	:	120 mA/cm <sup>2</sup>
•	Discharge voltage	:	1.1 V/cell, Av.
•	Battery voltage	:	13.2 V
•	Active electrode area	:	400 cm <sup>2</sup>
•	single cell power	:	~ 53 W
•	Stack/battery configuration	:	12S2P
•	Power from stack	:	~ 1 kW

•	Energy capacity	:	1 kWh
•	Charge capacity	:	~ 75 Ah





(Typical surface morphologies of electrode)

(170 kW/1 MWh unit, Sumitomo electric industries in Japan; Open Source)

The design of the above battery pack is in-line with the requirement for home light systems given by India Renewable Energy Development Agency (IREDA). The required battery by IREDA is 12.8 V and 80Ah (~ 1 kWh).



#### Dr. Anil Verma Professor

Indian Institute of Technology, Delhi Email: anilverma@iitd.ac.in

Dr. Anil Verma did his B.Tech. and M.Tech. from H.B.T.I. Kanpur. He worked in R&D of Asian Paints Ltd. He has completed his PhD from IIT Delhi. He joined IIT Guwahati in 2005 and thereafter joined IIT Delhi in 2015. He is working in the area of Electrochemical Engineering from last 19 years. His research work is focused on renewable energy and environment technologies. He is working on various Energy Conversion devices such as fuel cells, electrochemical conversion of CO2 to value added products. His present focus is on redox flow batter for stationary applications. His research work is majorly funded by DST, SERB, CSIR, DBT, New Indigo Project, DAE, CRERE Saudi Arabia, ISRO etc. He has published more than 75 pear reviewed papers in high impact, along with 9 book chapters and monographs. Guided 10 PhD students and filed 5 patents and has been granted 1 patent. He has received many awards including Amar Dye Chem Award by IIChE, UKIERI Research Fellowship award to pursue research in Newcastle University, Newcastle upon Tyne, UK. He was also a visiting Professor of Washington University in St. Louis in 2017.

**Compendium on MES 2018** 

## Metal Organic Material (MOM Embedded Electrospun Carbon Nanofiber (CNF) For Symmetric And Asymmetric Supercapacitor

## Aim

The objective of this proposal is to develop large scale production of cost-effective flexible supercapacitor with high energy density and power density. The electrode materials will consist of either a composite of metal-organic materials with carbon nanofiber or metal-organic derived metal embedded heteroatom doped graphitized carbon matrix with flexible carbon nanofiber.

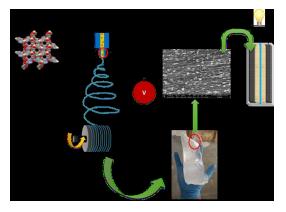
## Methodology

This project has three significant stages for fabrication of symmetric and asymmetric supercapacitors, namely- synthesis of MOM followed by fabrication of large-scale CNF/MOM composite for electrode fabrication, development of supercapacitor assembly with the upgraded electrodes and prototype development. A major emphasis will be laid upon development of upgraded material which exhibit large supercapacitance and composite fabrication. The final goal of the proposed research is an efficient solution for energy storage problem and prototype development.

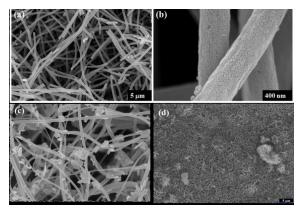
## **Expected Outcome & Deliverables**

- Novel Metal Organic Materials (MOM) synthesis for high energy and power density supercapacitor electrode.
- Facile and cost-effective synthesis of MOM/Carbon Nanofiber (CNF)
- Composite materials via Electrospinning for binder free electrode

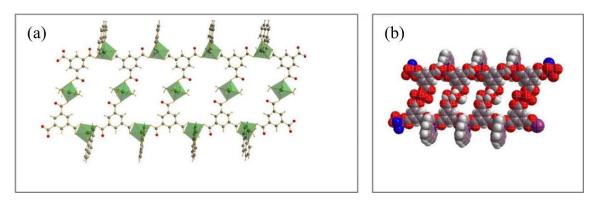
• Demonstration of capacitance of composite materials via two-electrode capacitor system



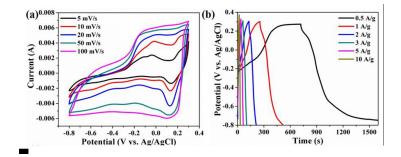
Graphical representation of the proposed objective of the study.



(a) and (b) carbon nanofibers (CNF), (c) MOF embedded polymer nanofiber network and (d) layered metal oxide nano-architecture.



(a) The molecular structure of Co-MOF (d) Space-filling model of Co-MOF.



## (a) CV data at different scan rates ranging from 5 to 100 mV/s, (b) Charge-discharge data at current densities ranging from 0.5 to 10 A/g with capacitance of 315 F/g



#### Dr. Rik Rani Koner Assistant Professor Indian Institute of Technology, Mandi Email: rik@iitmandi.ac.in

Dr. Rik has recived her PhD degree in Chemistry from IIT Guwahti. She is curently associated with IIT Mandi as an Assistant Professor in the school of Engineering. She has been working in the area of new multifunction hybrid materials inculeding metal-organic framework (MOFs), coordination polymers (CP) metal-organic gels (MOGs) for energy storage and energy conversion application.

# 12 Integrated Self-Powered Energy Storage System

## Aim

Design of materials to develop an integrated, self-powered energy storage system comprising nanogenerator and electrochemical supercapacitor.

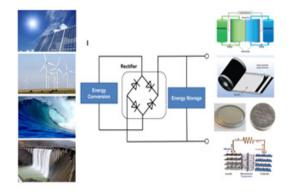
## Methodology

- To develop nanogenerator with optimized performance by materials selection and optimizing the composition in the nanocomposite.
- To study carbonaceous composite materials for electrochemical supercapacitors by optimizing pore structure and surface area.
- Coupling nanogenerator with electrochemical supercapacitor to demonstrate a prototype with self-powered charge/discharge.
- Synthesis and Characterization of new materials for dielectric and supercapacitors.

## **Expected Outcome & Deliverables**

 The concept of self-powered energy storage system using indigenously developed materials for nanogenerator and electrochemical supercapac -itor will be demonstrated using a prototype device





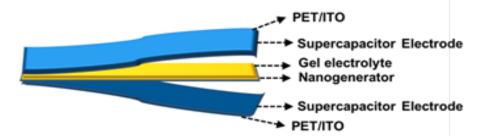
### Nanogenerator based on ZnO nanotubes





PET/ITO/ZnO(NT)/Al/ZnO(NT)/ITO/PET







Dr. N. Lakshminarasimhan Principal Scientist CSIR-Central Electrochemical Research Institute (CECRI), Karaikudi E-mail: laksnarasimhan@cecri.res.in ; nlnsimha@gmail.com

Dr. N. Lakshminarasimhan obtained his Ph.D. in Chemistry from Indian Institute of Technology (IIT) Madras, Chennai in 2005. Further, he carried out his postdoctoral research work at Pohang University of Science and Technology (POSTECH), Republic of Korea before joining CSIR-CECRI in 2009. He is a recipient of CSIR Young Scientist Award in Chemical Sciences for 2012. His broad research area is solid state chemistry and materials science. His research focuses on functional materials for energy and environmental applications. The materials of his interest include photofunctional materials (phosphors, photocatalysts, and photoanodes for DSSC), electrochemical energy storage (batteries and supercapacitors) and electroceramics (dielectric and magnetic materials).

## **13** High Energy Density Sodium-Ion Batteries Using Alluaudite And Mixed-Polyanionic Class Of Cathode Materials

## Aim

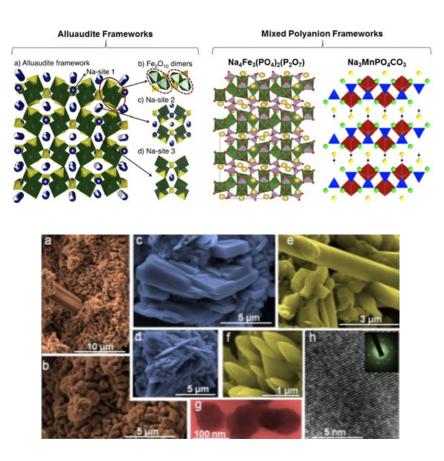
Synthesis of novel alluaudite  $[Na_2-xM_2(XO_4)_3]$  and mixed polyanionic cathode materials for Na-ion batteries.In-depth crystal/ magnetic structure analysis and Rietveld refinement of these novel compounds by combining powder X-ray, neutron and synchrotron diffraction. To optimize these new cathode materials to get energy density over 320-350 Wh/kg for practical large-scale use. Development of thin film micro-batteries using pulsed laser deposition. Demonstration of 18650 and pouch cell prototypes using these new cathodes and hard-carbon anodes.

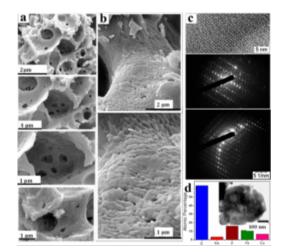
### Methodology

This project will focus on discovery of new cathode materials and exploration of newly discovered alluaudite and mixed-polyanionic cathodes for large-scale sodium-ion batteries. Unraveling new materials will be the cornerstone of the project. The structural features will be investigated using X-ray, synchrotron and neutron powder diffraction routes. Based on the earth-abundant elements, these economic cathodes will be employed in thin-film bateries and 18650 and pouch cells delivering energy density of 310-350 Wh/kg.

## **Expected Outcome & Deliverables**

- Discovery of new alluaudite and mixed polyanionic cathodes for economic large-scale sodium-ion batteries.
- Detail knowledge of structural, thermal and electrochemical properties performance of these new economic cathodes.
- Investigation of crystal and magnetic structures of novel cathodes for sodium-ion batteries.
- Optimization, development and demonstration of 50 numbers of 18650 type sodium ion cells with 2400 mAh capacity.
- Demonstration of thin film micro-batteries by PLD deposition.







Dr. Prabeer Barpanda Assistant Professor Indian Institute of Science, Bangalore E-mail: prabeer@iisc.ac.in

Prabeer Barpanda is currently serving as an Assistant Professor in the Materials Research Center at Indian Institute of Science (IISc), Bangalore. He completed his B. Engg. from National Institute of Technology Rourkela (NITR-India, 2002), M. Phil. from the University of Cambridge (UK, 2004) and Ph. D. from Rutgers University (USA, 2009). Following, he pursued postdoctoral work in the Universite de Picardie Jules Verne (France, 2009-2010) and the University of Tokyo (Japan, 2011-2013). Prabeer's research revolves around synthesis, structural and electrochemical study of novel materials for secondary Li-ion/ Na-ion batteries and supercapacitors. So far, he has published 106 journal articles, 42 conference proceedings and 3 world patents. He has received several awards including Shell Centenary British Chevening Fellowship (UK), C.G. Fink Fellowship (ECS, USA), H.H. Dow Award (ECS, USA), JSPS Postdoctoral Fellowship (Japan), ECS Young Investigator Award (2016), ISE Prize for Applied Electrochemistry (2016), Ross Coffin Purdy Award (ACERS, USA), INSA/NASI Medals for Young Scientists (2016) and IEI Young Engineer Awards (2015). He directs Faraday Materials Laboratory (FAMAL) at IISc.

## Studies On The Strength And Durability Of ZnO Nanowire / T1000 Carbon / Epoxy Composites For Flywheel Energy Storage

### Aim

The goal of the project is to improve the tensile strength, stress rupture, fatigue life and fracture toughness of T1000 carbon/epoxy composite flywheel material by at least 30% so that it can rotate faster. The specific objectives are:To fabricate ZnO nanowire / T1000 carbon / epoxy hybrid composites and study its mechanical properties. The properties of interest are interfacial strength, tensile strength and stiffness (normal & transverse), tensile stress rupture, fatigue life and Mode-I fracture toughness. To fabricate prototypes of composite flywheels (25cm length x 25cm OD x 2.5 mm thickness) and perform spin-test to determine the burst speed and energy density.

### Methodology

The approach is to integrate ZnO nanowires at the fiber/matrix interface (by hydrothermal method) in T1000 carbon/epoxy composites to increase the multidirectional properties and durability of flywheel composites, so that they rotate faster and thereby gain energy density. Laboratory scale coupon tests will be conducted to study the strengthening, durability and delamination failure of composites. Thin cylindrical composite flywheel prototypes (25cm length x 25cm OD x 2.5 mm thickness) will be fabricated by resin transfer molding (RTM) and subjected to spin-tests to determine their burst speeds and energy density. The proposed approach is a novel attempt to increase the strength and hence the energy density of flywheel composites, and such studies have not been conducted at the international as well as national levels.

## **Expected Outcome & Deliverables**

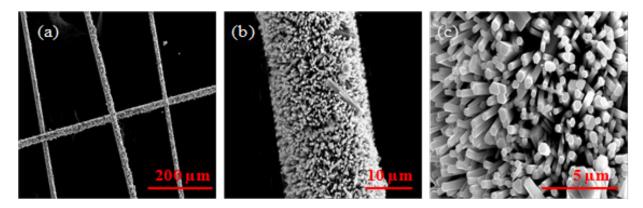
- Novel ZnO nanowire/T1000 carbon/epoxy hybrid composite flywheel materials with at least 30% improvement in tensile strength, stress rupture, fatigue life and fracture toughness.
- Database on the properties and guidelines on strengthening, durability and damage tolerance of ZnO nanowire/T1000 carbon/epoxy composites useful for flywheel designs.
- Thin cylindrical flywheel prototypes made of proposed hybrid composite materials .



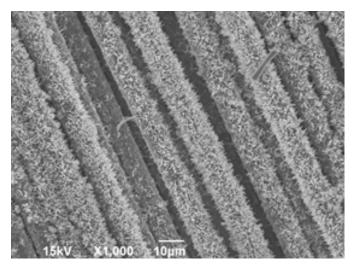
Porsche 911 GT3R with carbon fiber flywheel



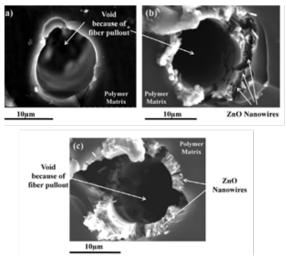
Carbon fiber flywheels for grid regulation



Fibers coated with ZnO nanowires



Fabrics coated with ZnO nanowire



Mechanical interlocking provided by nanowi



Dr. S. Gowthaman Assistant Professor IIITDM Kancheepuram, Chennai Email: gowthaman@iiitdm.ac.in

Dr S Gowthaman has about 15 years of research experience in the areas of experimental solid mechanics, composites and nanomaterials. He obtained his MS and PhD from North Carolina A&T State University, USA and did his Post-Doctorate research in Nanyang Technological University, Singapore. He has worked in projects sponsored by various agencies like NASA, US Army, ONR (USA), Wright Materials Research (USA), DSTA (Singapore), DST (India) and DRDO (India). To his credit, he has published more than 25 research papers in international journals and conference proceedings. His research focuses on providing solutions to structural needs in different applications.

## **15** Sulphur Nanoparticles Reinforced Hierarchical Assemblies Of Carbon Nanotubes For Efficient Lithium-Sulphur Batteries

## Aim

Development of Lithium-Sulphur Battery technology by using novel 3D structures made up of hierarchical assemblies of CNTs. Effective encapsulation of Sulphur in between CNT bundles so that volume expansion of S can be controlled, migration of polysulphides can be mitigated and high performance Li-S battery with capacity reaching the oretical capacity with improved cyclability can be demonstrated.

## Methodology

The objectives of the project will be achieved by using several nanofabrication, characterization and electrode designs. CNTs grown on patterned catalyst will be used to form 3D structures. In-situ densification process will be utilized to trap Sulphur nanoparticles in between vertically aligned CNTs. Synthesis and characterization of nanostructures (CNT/S) will be done by FESEM, TEM, Raman and XRD. Lithium-ion cells in the form of coin cell and large area pouch cell will be assembled and later electrochemical characterizations will be performed.

## **Expected Outcome & Deliverables**

- Development of electrode design for high performance Li-S battery with Capacities reaching theoretical capacity.
- Improved cyclability of more than 100 cycles with capacity of more than 1000 mAh/g is expected which is much better than most of the reported Li-S batteries.

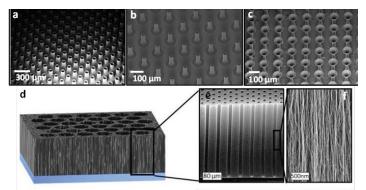
- Intoduction of several novel approach for electrode fabricaiton that could benefit the researchers in the field of energy storage.
- Demonstration of conventional coin-cells as well as large area pouch cell Li-S battery with up to the mark battery performance.



Central government had launched a flagship scheme called 'Faster Adoption and Manufacturing of Electric Vehicles' (FAME) to give a spur to the electric vehicle industry in India, and under it, financial assistance is being provided to electric vehicle manufacturers till 2020 for building infrastructure and R and D facilities. Image Credit: https://greentechlead.com/

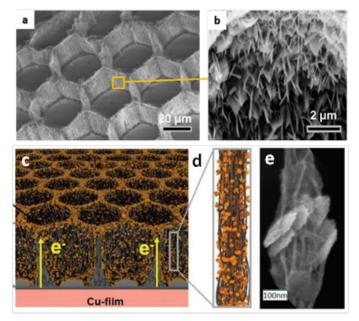


Bangalore-based Ather launched electric two wheelers, the Ather 340.



CNT Micro and Nano-structures

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Hydrothermal coating of CNT Honeycomb Micro and Nano-structures



#### Dr. Shahab Ahmad Assistant Professor Indian Institute of Technology, Jodhpur Email: shahab@iitj.ac.in

Dr. Shahab Ahmad hold PhD in Physics [2014] from Indian Institute of Technology-Delhi with thesis entitled "Fabrication and Optoelectronic Studies of Inorganic-Organic Hybrid Semiconductors". After PhD he moved to the University of Cambridge (UK) to work as Post-Doctoral Research Associate on Energy Storage (Li-ion Batteries) and Optoelectronic (Perovskite Solar Cells) devices, for duration of 3 years [2014-2017]. He returned to India to join Assistant Professor at Centre for Nanoscience and Nanotechnology, Jamia Millia Islamia, JMI (Central University), New Delhi, India [2017-2019]. Recently he took up the position of Assistant Professor at Department of Physics, Indian Institute of Technology Jodhpur. Dr. Shahab Ahmad has post-PhD research experience of more than 5 years and is author of 33 research articles. During post-doc in group of Dr. Michael de Volder at Cambridge he worked on energy storage devices including ultraflexible and stretchable Li-ion batteries, ultrathick electrodes. He integrated his previous expertise on perovskites with energy storage devices and worked out a unique device known as a Photo-battery. At Cambridge, he also worked in close collaboration with Prof. Jeremy Baumberg (FRS) and Prof. Sir Richard Friend (FRS) at Cavendish Laboratory on various research aspects of metal halide perovskites ranging from LEDs, Solar cells to Solar water-splitting applications. His key publication includes Advanced Materials, Advanced Energy Materials, Nano-Letters, ACS Nano, Small, ACS Applied Materials and Interfaces, JAP etc. His current research interest includes Photo-Rechargeable, Flexible and Stretchable Energy Storage Devices, Optoelectronics and Spectroscopy of Metal Halide Organo Perovskites, Solar Cells, Photo-Detectors, LEDs, Solar Water Splitting-H2 production, Advanced Functional Nanomaterials.

**Compendium on MES 2018** 

# Earth Abundant Metal Based Electrode Materials For Energy Storage Applications

## Aim

- To synthesize materials/composites that would improve the performance and decrease the cost of energy storage devices.
- To increase the energy density and power density of earth abundant metal based Na+/K+ ion capacitors.
- Using the as mentioned nanomaterials/composites, the benchmark power densities (~ 100 Wh/kg) and energy densities (~20000 W/kg) would be achieved.

## Methodology

The initial modus operandi would be modification (selective surface termination and control of morphology) of the electrode materials that have been already reported as electrode materials for Na+, K+ and Al3+ ion batteries.

Our group's expertise in micro- emulsion, hydrothermal, as well as high temperature synthesis methods would be an asset. Based on the results obtained, systematic variation in composition would be carried out to evaluate newer materials for the target application. The following classes of materials would be evaluated (1) Oxide based materials including titanates and niobates (b) Ti3C2 and related MXenes (c) Layered double hydroxides and (d) phosphorenes.

## **Expected Outcome & Deliverables**

The following novel electrocatalysts will be synthesized

- Different morphologies of Sodium titanates, vanandium oxides, Niobium and Nickel/Cobalt oxides and their composites with 2D materials (rGO and MoS2).
- Different morphologies of Ti3C2 and similar MXenes.
- Phosphorene nanocomposites with 2D materials.Na+) during the operation of the device.

Using these nanomaterials/composites, we hope the benchmark power densities (~ 100 Wh/kg) and energy densities (~20000 W/kg) would be achieved.

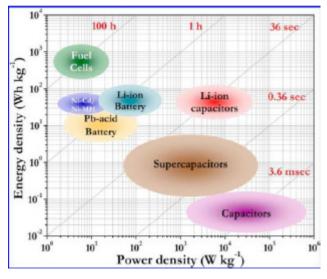
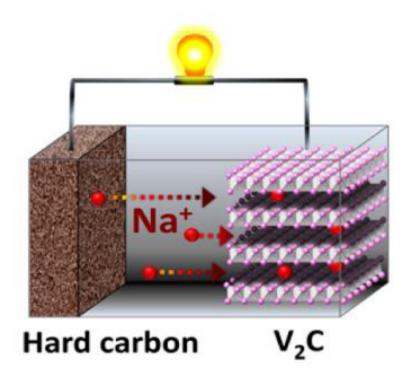


Figure 1: Ragone plot depicting the energy and power densities of reported electronic energy storage devices. Ref: Chem. Rev. 2014, 114, 11619.



A new electric bus based on supercapacitor technology was put into operation in China in 2015. It is capable of achieving full charge in 10 seconds.



Cathode EDLC Type Positive Anode Battery Type /Faradaic (intercalation principle)

An Ion capacitor, one electrode is battery type (intercalation) and another is capacitor type.

The high cost of Li metal used in Li ion based batteries necessitates the exploration of cheaper alternatives

- Recently earth abundant metal (Na+, K+, Al3+) based systems (henceforth called ion capacitors) have been theoretically predicted and experimentally achieved. There are several reasons that facilitate these ions for being suitable candidates for replacing Li+ in these ion capacitors.
- The standard Na/Na+ potential of -2.714 (vs SHE) is close to that of Li/Li+ (-3.04 vs SHE).
- Na based non-aqueous electrolytes generally exhibit ionic conductivities, an

electrochemical window and stabilities comparable to Li ion counterparts.

- Divalent (e.g. Mg2+) and trivalent (e.g. Al3+) ions result in multiple electron generation per cation, hence devices with electrodes based on these ions are expected to perform better in terms of both energy and power density.
- The bottleneck in development of these devices arises from the lack of a propriate materials that allow fast intercalation of the relevant ions (e.g. Na+) during the operation of the device.



Dr. Ashok Kumar Ganguli Professor Indian Institute of Technology, Delhi Email: ashok@chemistry.iitd.ac.in

Professor Ashok Kumar Ganguli is currently the deputy director, strategy and planning, a Institute Chair Professor and Professor of Chemistry (HAG) at IIT Delhi. He is the founding Director of Institute of Nano Science and Technology in Mohali (Jan 2013- Jan 2018). Prof. Ganguli obtained his Ph.D. degree from the Solid State & Structural Chemistry Unit (SSCU) of Indian Institute of Science, Bangalore in 1990 in the area of Thallium based high temperaturesuperconductors for which he got the Sudborough Medal of Indian Institute of Science. He has been a visiting scientist at Dupont Company, USA (1990-91) and a postdoctoral associate and visiting scientist at Ames Laboratory, Iowa State University, USA (1991-93 and 2004-05). His areas of interest are in the design of nanostructured materials for applications in water purification, solar energy conversion and microfluidic devices and also high temperature superconductivity. He has published over 250 papers and has filed five patents.

## Mitigating Dendrite Growth Using Engineered Electrolyte Layers For The Development Of High Energy Density, Long Cycle Life Lithium Batteries

## Aim

To enable the lithium metal as anode for rechargeable lithium-ion battery systems by mitigating the dendrite growth and thereby stabilizing lithium electrodeposition by

- By generating electrostatic shield mechanism on lithium anode surface using certain organic/inorganic additives.
- By forming artificial solid electrolyte interface Artificial Solid Electrolyte Interface (A-SEI) on the anode surface.
- By developing nanoporous solid state electrolyte membranes with tethered anions.

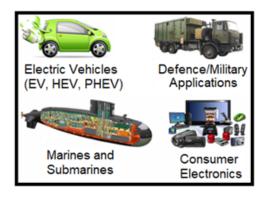
## Methodology

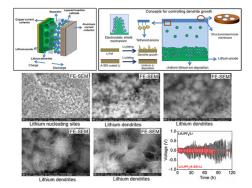
The focus of the proposed research plan encompasses R&D activities in the following research aspects

- To use certain organic/inorganic electrolyte additives that has lower effective reduction potential, when compared to the standard electrode potential of lithium-ion, in the anode/electrolyte interface, providing a self-healing electrostatic shield mechanism for controlled electrodeposition of lithium during electrochemical cycling in Li/Li symmetric cells.
- The proposed technology also involves the preparation of anion tethered nanoporous solid state electrolytes to overcome the uncontrolled lithium electrodeposition in Li/ Li symmetric cells.
- Fabrication and electrochemical characterization of lithium metal batteries using various cathode materials viz. Lithium Iron Phosphate (LFP), lithium nickel manganese cobalt oxide (NMC) and Molybdenum sulfide (MoS<sub>2</sub>).
- Performance characteristics in cylindrical cells .

## **Expected Outcome & Deliverables**

- Introduction of unique electrode/electrolyte interface design that can control/ mitigate the dendrite growth in lithium anode based batteries.
- Design and fabrication of lithium anode based cylindrical cells that can render high energy density and long cycle life.
- To make global visibility of VISTAS and India in lithium anode based battery research.







Dr. A. M. Shanmugharaj Assistant Professor Vels Institute of Science, Technology & Advanced Studies (VISTAS), Chennai Email: a.m.shanmugharaj@gmail.com

Dr. A. M. Shanmugharaj received his Ph. D degree from "Rubber Technology Centre, Indian Institute of Technology", Kharagpur in 2004. Then, he joined "Department of Chemical Engineering, Kyung Hee University, South Korea" as postdoctoral fellow/associate scientist to work on the development of polymer nanocomposites and controlled living radical polymerization reactions. In 2006, he joined as research associate in "Institute of Materials Chemistry and Engineering (IMCE), Kyushu University", Japan to work on polymer based UV resistant coatings. In 2007, he got the JSPS postdoctoral fellowship to carry out research work on ferroelectric nanocomposite films and continued the position upto December, 2008. After one year industrial experience in "Phillips Carbon Black Ltd, Durgapur" as Manager-Product Development, he joined as "Assistant Professor" in the "Kyung Hee University, South Korea in 2010. During this tenure, his research areas were focused on the synthesis of nanomaterials for energy storage applications including batteries and supercapacitors, nanocatalyst materials for hydrogen production, self-healing polymers and its nanocomposite. After his 7 years tenure in South Korea, in 2017, he joined VISTAS as "Associate Professor/Senior Scientist" and associated with the "Centre for Energy and Alternative Fuels". His current research interest focused on the development of novel materials for battery applications, mitigating dendrite growth in lithium anodes, self-healing polymeric binders for silicon based anodes and nanocomposite materials for anti-corrosion coatings.

## **10** Development Of Lithium Ion Battery Module From Recycled Battery Materials For Stationary Applications

## Aim

Development of cathode and anode from recycled material. Electrochemical, thermal and structural characterisation of electrode materials. Feasibility study of Liion battery made with electrode from mixture of recycled and virgin materials.

## **Methodology**

Used Li-ion batteries will be recycled using simple, cost efficient and environmental friendly technologies. Recycled cathode material in form of Li complex will be evaluated as cathode material for new battery. Recycled graphite to be evaluated as an anode electrode. Structural and electrochemical characterisation will be carried out on the recycled electrode materials. Anodes and cathodes from these recycled materials will be fabricated. Their individual electrochemical performance in a half cell configuration against Li metal will be evaluated. In second part of project (if extended), a full cell in pouch type of configuration will be fabricated with stacked electrodes to achieve 50 Ah to 70 Ah capacities. The battery module along with necessary thermal management system will be developed and the entire module will be validated for India specific conditions.

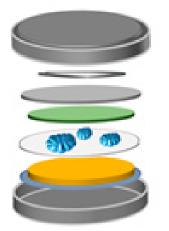
## **Expected Outcome & Deliverables**

• Development of recycled material that can be used in production of electrodes for new battery.

- A new study on feasibility of developing new Li-ion batteries from recycle materials.
- Development of a battery module, consisting of cells made from recycle material, along with thermal management system for household application (extended part).



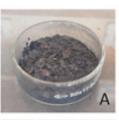
Discarded Car Batteries used as Stationary Power Source.



Top cap Spring Spacer Anode Electrolyte Separator Cathode Bottom cap

Structure of a Coin Cell





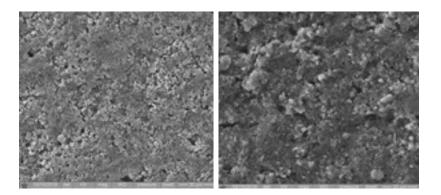


Coin cells fabricated from recycled anode (A) and cathode (C) material

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SEM Image of Electrode Made from Virgin Cathode Material (Left) and Recycled Cathode Material (Right).



Dr. Manjusha V. Shelke Principal Scientist CSIR-National Chemical Laboratory (CSIR-NCL), Pune E-mail mv.shelke@ncl.res.in

Manjusha Shelke is a Principle Scientist at CSIR-National Chemical Laboratory, Pune in India. She is a materials' chemist and works on development of high energy electrode materials and flexible platforms for energy storage devices like rechargeable batteries (Li-ion, Li-sulphur, Na-ion) and supercapacitors. Manjusha has PhD in chemistry from CSIR-Advanced Materials and Processes Research Institute, Bhopal, MP, India. She had worked as visiting researcher at Institut d'électronique de microélectronique et de nanotechnologie (IEMN), Lille, sponsored by Embassy of France in India in 2007-08 and at Rice University, Houston, TX, USA sponsored by Indo-US Science & Technology Forum (IUSSTF) in 2013-14. She has been selected as Kavli Fellow by National Academy of Sciences (NAS), USA in 2015 and as a Fellow of Maharashtra Academy of Sciences (MAS) in 2018.

## Virtual Energy Storage Based Demand Response Algorithm To Enhance The Performance Of Battery Energy Storage In Smart Grid

## Aim

To model the refrigerators and air conditioners (having time constant more than 30 minutes) analogous to battery which generates the virtual energy storage capacity. Hence it enhances the lifetime of the battery storage by preventing deep discharge of batteries.

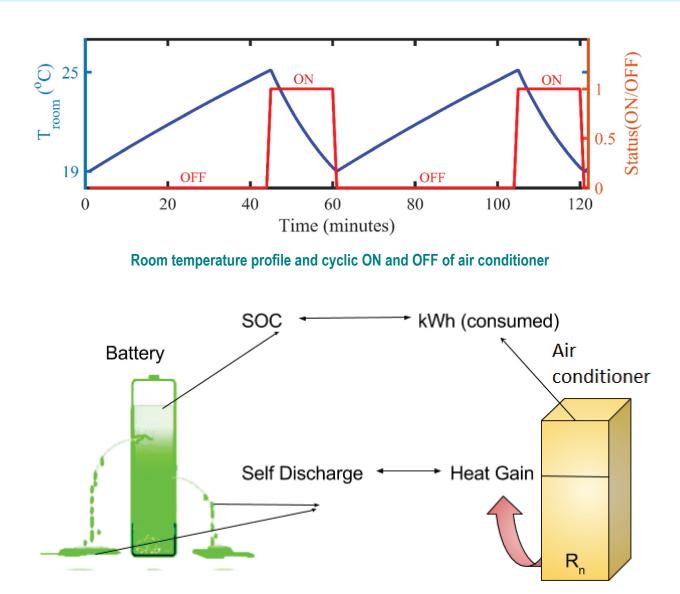
## Methodology

Emerging smart cities would have increased penetration of renewable resources which requires huge Energy Storage (ES) to ensure the reliability and stability of the system. Loads with large time constant i.e. more than 30 minutes in smart city such as refrigerators and air conditioners are identified as an alternative Energy Storage; which are modelled as thermal loads with cyclic or varying pattern of ON and OFF cycles. These loads are modelled analogous to the electrochemical batteries having virtual energy storage capability in the form of thermal energy. Artificial Intelligence (AI) based models will be developed to model the refrigerators and air conditioners of the smart city to estimate the virtual energy available in the residential loads. A Demand Responsibility Management (DRM) algorithm will be developed to dispatch the Virtual Energy Storage (VES) and Energy Storage in real time which encourages the utilization of the renewable energy locally resulting in an efficient system. The algorithm allows the 100% utilization of Energy Storage as Virtual Energy Storage supplies beyond the maximum allowable Depth of Discharge (DoD) of major Energy Storage technologies (e.g. 80% Depth of Discharge). Further, Demand Responsibility Management algorithm based on Virtual Energy Storage prevents deep discharge

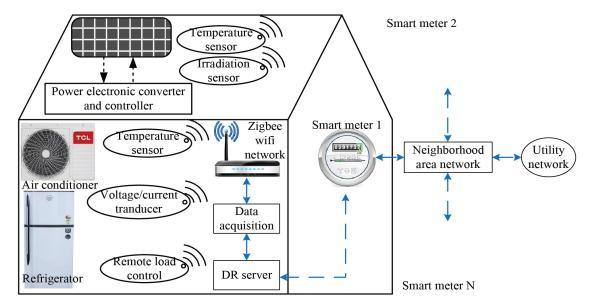
cycle of battery Energy Storage (ES) which enhances the battery lifetime.

### **Expected Outcome & Deliverables**

Al based demand response algorithm that estimates that the VES in the smart grid and dispatches the VES and ES in real time. Further, a laboratory based prototype that validates the proposed algorithm based on the concept of VES.



Analogy of air conditioner as electro-chemical battery



#### System Architecture for Study



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ManjushaDr. Vijayakumar K obtained his Bachelor's Degree in Electrical and Electronic Engineering in the year 2006 from Coimbatore Institute of Technology, Coimbatore. He secured All India Rank 358 in GATE exam and obtained his M.Tech. in Power Systems and Ph.D. from National Institute of Technology, Tiruchirappalli. He also selected for Canadian Commonwealth Fellowship-GSEP at University of Saskatchewan, Canada during his Ph.D. Further, He was a Postdoctoral Research Fellow in Nanyang Technological University, Singapore. POSOCO-2014 Awardee for Doctoral category and listed his Ph.D. dissertation in top 10 among all IIT's and NIT's in the year 2014. Dr. Vijayakumar is currently working as faculty in the school of Computer and Electrical Engineering, Indian Institute of Information Technology, Design and Manufacturing, Kancheepuram, Chennai. He was an Assistant Professor in the Department of Electrical Engineering, Malaviya National Institute of Technology, Jaipur, Rajasthan, India in the year of 2013-2018. He received Young Scientist Award for Start-up research grant which was given by SERB - DST in the year 2015. He is also the Young Faculty Fellow of Ministry of Communications & Information Technology. He was a Visiting Professor at University of Saskeatchewan, Canada and fellow of Indo- Canadian shastri Institute.

## **20** Facile Synthesis And Development Of 3D -Graphene/ WS<sub>2</sub>/Oxydized-Cnt Nanohybrids As Advanced Electrode Materials For High Performance Flexible Supercapacitors.

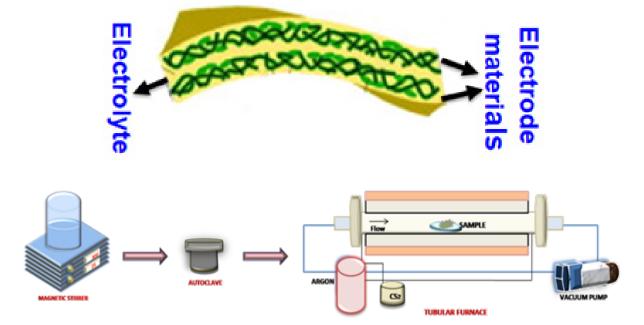
## Aim

To synthesis 3D-graphene modified  $WS_2$  and oxidized CNT nanohybrid electrodes for supercapacitor application. Synthesis of novel ionic liquid based polymer electrolytes (IL-b-PE) and their applications in flexible supercapacitors. In this case, ionic liquid based polymer electrolyte (IL-b-PE) will be act as electrolyte and as well as separator.

## **Methodology**

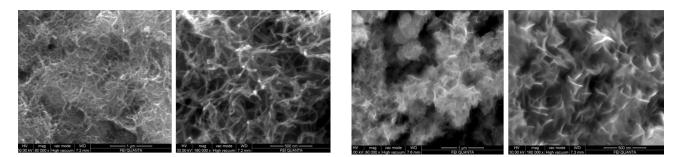
The electrode materials will be synthesized by hydrothermal method followed by heat treatment in CS2 environment.

## Flexible supercapacitors



## **Expected Outcome & Deliverables**

- Flexible supercapacitor device (can be bent, distorted, knotted or stretched without obvious cracking or flaking) will be developed.
- Development of low cost WS<sub>2</sub>/rGO/CNT composite electrode for supercapac -tor application.
- Novel ionic liquid based polymer electrolytes (IL-b-PE) and their applications in flexible supercapacitors. In this case, ionic liquid based polymer electrolyte (IL-b-PE) will be act as electrolyte and as well as separator.
- Prototype flexible device based on synthesized supercapacitor electrodes and ionic liquid based polymer electrolytes.
- Intellectual property right, if any.



Nanostructured WS2 electrode materials for flexible supercapacitor



#### Dr. Manab Kundu Research Assistant Professor SRM Institute of Science and Technology, Tamil Nadu Email id: manabm@srmist.ac.in

Dr. Manab Kundu received his Ph.D. in the field of Lithium-ion battery from CSIR-Central Glass and Ceramic Research Institute, Kolkata in 2012. After his PhD, he worked as postdoctoral researcher at International Iberian nanotechnology Laboratory (INL), Portugal,National University of Science and Technology (MISISNUST) Moscow, Russia and Norwegian University of Science and Technology (NTNU), Trondheim, Norway. He is presently supervising 3 Ph.D. and several M.Sc students. His current research is focused on nanomaterial synthesis, flexible supercapacitor and metal-ion battery.

## **Design And Development Of 2-D Sns Based** Nanostructures Coupled With Plasmonic Sn Nanosheets For Supercapacitor Application

## Aim

The prime objective of the project is design and development of 2-D SnS based nanostructures coupled with plasmonic Sn nanosheets for supercapacitor applications.

## **Methodology**

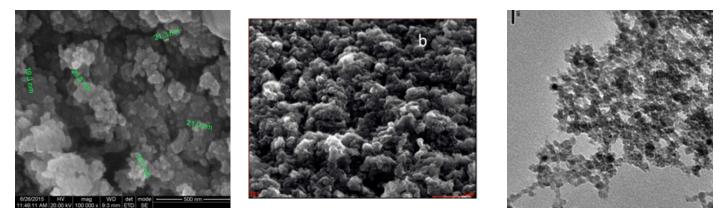
- 2D SnS nanostructures coupled with plasmonic Sn nanosheets (hybrid) is a unique design which can show enhanced super capacitor performance compared to pure 2D-nanostructures by harnessing the light energy.
- The incorporation of metal nanostructures, especially Sn nanosheets will enhance the conductivity of the electrode.
- The plasmonic effect of Sn nanosheets can be harnessed to improve the energy storage capability of the super capacitor.
- Light induced energy storage assisted by the plasmon coupled 2D nanostructures is a least explored and novel area with promising possibilities.

## **Expected Outcome & Deliverables**

Novel design and development strategy for light assisted 2D- plasmonic super capacitor electrode material with

- High mass specific capacitance ~ 1500 Fg-1
- High current density ~ 3A/g-1
- Columbic efficiency of 100%
- Stability for minimum of ~ 2000 cycles.

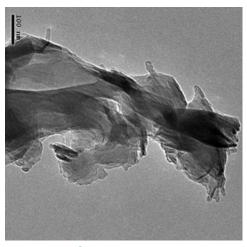
 10 to 50% light assisted enhancement in electrochemical performance of the fabricated



Tin sulphide nanostructures

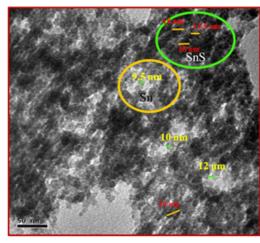
2-D Sn nanoparticles

**Compendium on MES 2018** 



**Sn-Nanosheets** 

Dr Anita R Warrier



**SnS-Sn nanohybrid structures** 



Assistant Professor AMET University (Academy of Maritime Education and Training), Chennai Email: anitawarrier2@gmail.com

Dr. Anita Warrier received her Ph.D. in Physics from Cochin University of Science and Technology in 2011. Then joined Department of Physics as Post-doctoral fellow till 2014. She is presently Associate professor at Academy of Maritime Education and Training (AMET University)She heading several research projects sponsored by DST, DAE-BRNS and CSIR. She is presently supervising 4 Ph.D. and has guided several B.Tech and M.Tech students. Her current research is focused on nanophotonic materials for energy and environment applications, photothermal techniques for non-destructive testing.

# **Development Of Low Cost, Long Cycle Life** Sodium-Ion Batteries For Grid Energy Storage

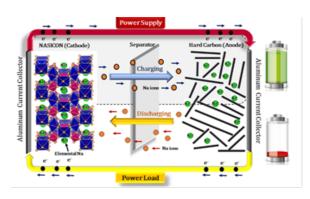
#### Aim

- To develop high energy density (150 Wh kg-1) sodium ion batteries (NIBs) and demonstrate at least 2000 stable cycles at 1 C rate in coin cell configuration (4 mAh).
- To accelerate the discovery of next generation electrode materials through joint efforts of computational and experimental studies.
- To explore low cost and energy efficient synthesis routes.

#### Methodology

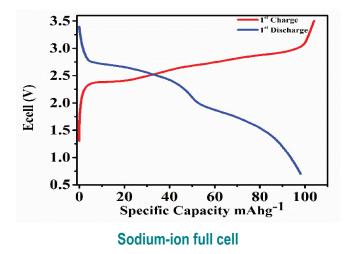
This proposal aims to build low cost, long cycle life NIBs through a two-tier approach, i.e. one focuses at materials level and another at system level. Inexpensive and non-toxic cathodes will be developed based on the guidelines from DFT calculations.

Advanced high energy density anodes will be realized through integration of hard carbon and alloy elements. The as-developed electrodes will be subjected to various structural, morphological and electrochemical studies to understanding the underlying reaction mechanism followed by performance optimization in half cells. The down-selected candidate will be assessed further in full Na- ion cells with systematic protocols and benchmarked against the state-of-the-art materials using technoeconomic modeling.



#### **Expected Outcome & Deliverables**

- The DFT guided experimental approach is expected to result in finding of low cost and air stable layered oxide cathodes while our attempt to integrate hard carbon and alloy elements are targeted to increase the energy density of anodes.
- The systematic protocols on full Na-ion cells is expected address several issues originate during their operation and provide a fruitful pathway to achieve high energy density (150 Wh kg-1) and long cycle life (2000 cycles) NIBs.
- The corresponding results are highly expected to create new IPRs and get published in high impact journals.





SEM image of high capacity hard carbon-antimony composite



Dr. P. Senguttuvan Assistant Professor JNCASR, Bangalore Email: prem@incasr.ac.in

Dr. Premkumar Senguttuvan received his Ph.D. from Université de Picardie Jules Verne, Amiens, France in 2013. He worked as a Postdoctoral Appointee at Argonne National Laboratory from 2014 to 2016. He has wide range of expertise on material synthesis and characterization for modern rechargeable battery technologies.

# 23

Design And Testing Of Robust And Flexible 3D Printed Electrodes With Novel Porous Architecture Guided By Graph Theory And Molecular Simulations For High Energy Density Applications

#### Aim

Design and development of ion-specific pore architecture of carbon/ graphene-based electrode material for supercapacitors through graph theory and molecular simulations. Understand and tune the molecular interactions between the electrolyte and electrode materials at the nanoscale to achieve a high energy density b increasing the Electrochemical Stable Potential Window (ESPW). Analyze the effects of polymer additives and nanoparticles on the potential window, viscosity, conductivity and resistance of the electrolyte through experiments.3-D printing of the electrode with the novel porous architecture as dictated by theory and simulations.

#### Methodology

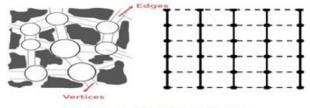
The focus lies in designing of porous electrodes by modeling each pore as vertices of a graph based on the data obtained from molecular dynamics simulations. We intend to get insights on transport properties like diffusion/adsorption using network/ connectivity analysis of graph theory. Amongst the pores with better connectivity, the best suited are chosen depending on the free energies obtained through molecular simulations. Electrode with novel porous architectures are then developed using 3D printing technology and their performance would be tested experimentally.

#### **Expected Outcome & Deliverables**

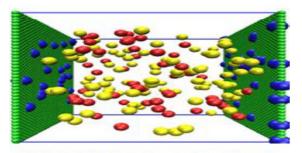
• Development of a three-dimensional porous architecture for electrode materials in supercapacitor applications which will have a high specific area,

higher connectivity and suited for high energy density applications.

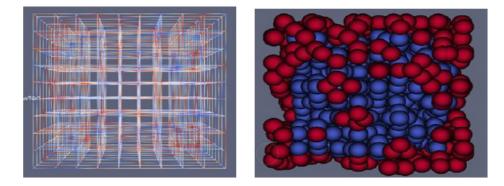
- Owing to their high robustness and flexibility, these are tailor-made for high energy-dense applications in defence, space and also in the biomedical sector.
- Develop a "pore simulator" that provides a 3D porous architecture with high connectivity and high specific capacitance for energy-dense applications and this GUI Graphic User Interface) is also intended to be used for educational and industrial applications.



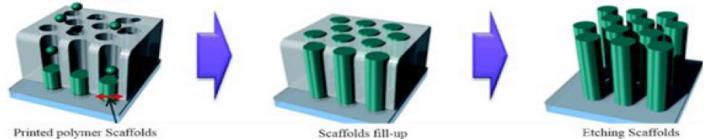
Graph Theory Aided Porous Model



Molecular Dynamics simulations to understand ion-specific interactions



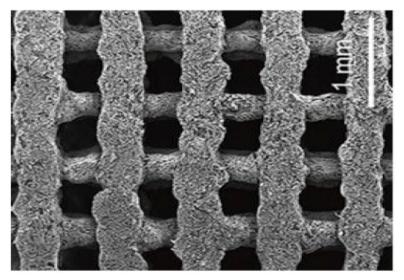
**3D Porous Network cross sectionl view** 



Printed polymer Scaffolds

Scaffolds fill-up

#### **3D Printing of the Porous Architecure**



3D Printed Graphene Lattice (image by Bin Yao)



#### Dr. Mithun Radhakrishna Assistant Professor, Indian Institute of Technology, Gandhinagar, Gujarat Email - mithunr@iitgn.ac.in

Dr. Mithun Radhakrishna recevied his Ph.D. in Chemical Engineering from Columbia University. During his Ph.D. he focused on understanding protein-surface interaction and the effect of surface curvature on protein stablity using simpel lattic models through Monte Carlo simulation. He worked as a Postdoctoral resarcher at the university of illinois at urbana-Champaing. He worked on charged polymer systems and tried to understand charge correlations and their effect on the phase behaviour and morphologies of these system using a combination of mean-feild theories and Gibbs Ensemble Monte Carlo Simulations. His group is intrested in the study of soft matter system (proteins, polymer, and a number of biologocal materials ) using the principles of Statistical Mechanis and polymer physics. His group uses a combination of theory and molecular simulations ( Monte Carlo and Molecular Dynamics ) to draw insights into the interaction that take place at the Nano-scale.

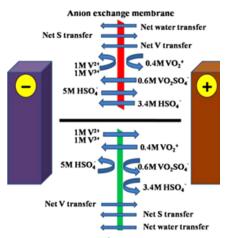
# **24** Indigenous Polymer Electrolyte Membranes For Energy Devices: Redox Flow Battery And Reverse Electrodialysis

#### Aim

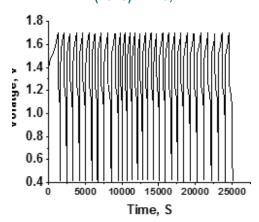
Design and Development of new generation ion-exchange membranes with excellent stability in acidic and alkaline environment; mechanical and thermal stability and electrochemical performance. The membranes with equivalent properties to that of Nafion® and Neosepta®. The comparative performance evaluation in redox flow battery specifically Zinc and vanadium redox flow battery. The development of alternative organic redox couple will be attempted.

#### Methodology

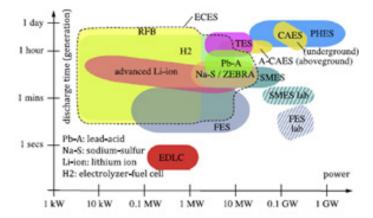
There are three different approaches to develop ion-exchange membrane with polymer backbone and structural resemblance to perfluorinated common polyelectrolyte membranes, Nafion® developed by DuPont, and Aquivion® The developed Solvay speciality polymers. first approach will by be interpenetrating polymer network, where functional monomers will be copolymerised with perfluorinated polymers. The second and third approach will be based on functional modification of perfluorinated polymers with suitable organic molecules to dock the ionic cluster on polymer backbone. The developed membranes will be thoroughly evaluated for their electrochemical and physicochemical properties. The developed membranes have plethora of applications in energy devices for generation and utilisation of green and clean energy.



lons and water transfer directions in typical vanadium redox flow battery with anion and cation exchange membranes, Electrochimica Acta 101 (2013) 27-40,



All iron alkaline redox flow battery performance with polyethylene based Interpolymer cation exchange



Power duration diagram of Different energy storage devices, (Renewable and Sustainable Energy Reviews 29, (2014) 325-335)



Cartoon showing utility of redox flow battery in greed applications with organic redox molecules for sustainable development. (Chem. Soc. Rev. 47 (2018) 8721-874)



Dr. Rajaram K Nagarale Senior Scientist

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Dr. Rajaram. K. Nagarale is MSc in inorganic chemistry (1999) from Karnatak University Dharwad with Prof. G. K. Narayanareddy gold medal for standing first followed by PhD (2006) from CSMCRI, Bhavnagar. Subsequently (2006), he worked as a post-doctoral fellow with Prof. Woonsup Shin at Sogang University, Seoul, Korea. Here, in 2008 he was made research professor in the department of chemistry and integrated biotechnology. In 2009, he joined Prof. Adam Heller of Chemical Engineering Department, University of Texas at Austin. Here, he along with Prof. Heller and Prof. Shin developed the non-gassing electrodes for the electro-osmotic pump based insulin delivery devices. In 2012, he received the prestigious 'Ramanujan Fellowship' and with the award he joined the Department of Chemical Engineering, Indian Institute of Technology Kanpur, under the mentorship of Prof. P. K. Bhattacharya and Prof. Ashutosh Sharma. In 2015, he joined as senior scientist at CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar-364002, Gujarat. During his research carrier of about 12 years, he has over 65 peer reviewed research publications and two issued patents. His main research interest at CSIR-CSMCRI is ion exchange membrane and their device applications.

# 25 Computational Design And Experimental Development Of Sodium-Ion Battery Materials And Technology

#### Aim

Computational and experimental design of high performance cathode and anode materials for Na-ion batteries. Optimize electrode fabrication process and scale-up the materials (100 g) to develop a proto-type Na-ion battery delivering capacity of 500 mAh and 2.5 V.

#### Methodology

Based on the computational design of electrode materials, scalable processes like sol-gel and solvo/hydrothermal process are adopted for material synthesis. The materials are further tested for its structural, morphological and electrochemical characterizations.

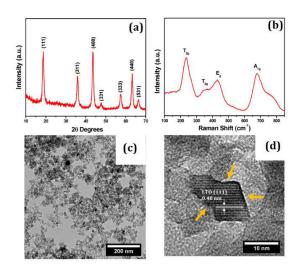
#### **Expected Outcome & Deliverables**

- First principle based computational design of new and advanced Na-ion battery electrode materials.
- Development of high performance anode and cathode materials experimentally.
- Scale-up of optimized material synthesis to 100 g in lab.
- Prototype full-cell pouch cell development delivering 500 mAh capacity with 2.5 V, wide temperature of operation and cycling stability to 500 cycles.
- Patents, publications and manpower generation.

#### Materials investigated so far

**Anode:** Lithium Titanate ( $Li_4Ti_5O1_2$ ), Sodium Titanate ( $Na_2Ti_6O1_3$ ) **Cathode**: Sodium Vanadium Phosphate ( $Na_3V_2(PO_4)_3$ )

#### **Structural & Morphological Characterizations**



#### Lithium Titanate (Li<sub>4</sub>Ti<sub>5</sub>O1<sub>2</sub>):

Fig. 1 (a) XRD, (b) Raman and (c & d) TEM images of  $Li_4Ti_5O1_2$  anode

#### Sodium Titanate (Na<sub>2</sub>Ti<sub>6</sub>O1<sub>3</sub>):

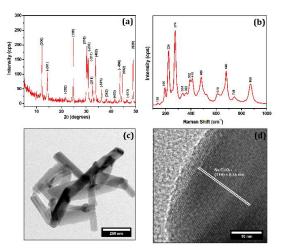


Fig. 2 (a) XRD, (b) Raman and (c & d) TEM images of  $Na_2Ti_6O1_3$  anode

#### Sodium Vanadium Phosphate $(Na_3V_2(PO_4)_3)$

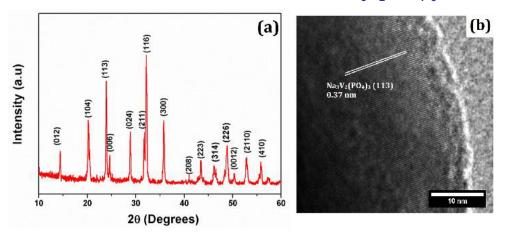


Fig. 3 (a) XRD and (b)) HR-TEM image of  $Na_3V_2$  (PO<sub>4</sub>)<sub>3</sub> cathode

Electrodes were fabricated as half-cells (with Na metal as counter/reference electrode) to test the electrochemical performance as sodium ion battery electrodes. Optimization were done to improve the electrochemical performances of each electrodes in terms of tuning material synthesis and electrolyte selection.

#### **Electrochemical Characterizations**

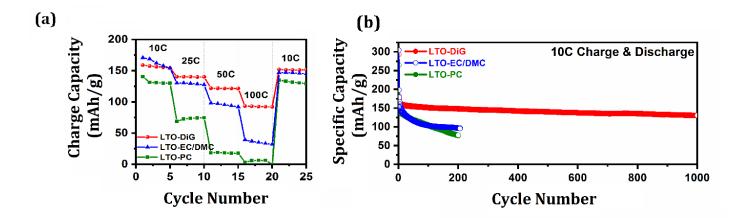
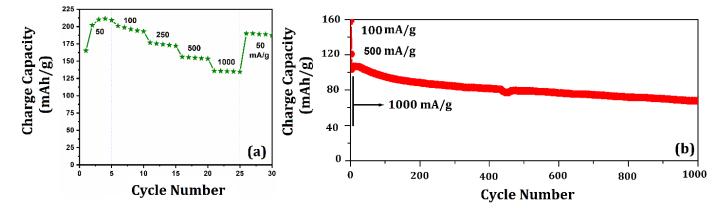
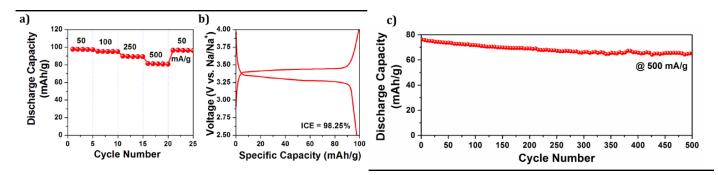


Fig. 4 Electrochemical performance results of LTO in 3 electrolyte formulation (a) rate performance from 10C to 10°C, 5 cycles each and (b) long cycling at 10°C rate.

Compendium on MES 2018







# Fig. 6 (a) Rate performance at different rates (b) charge-discharge profile at 50 mA/g and (c) long cycling at 500 mA/g of Na3V2(PO4)3 cathode



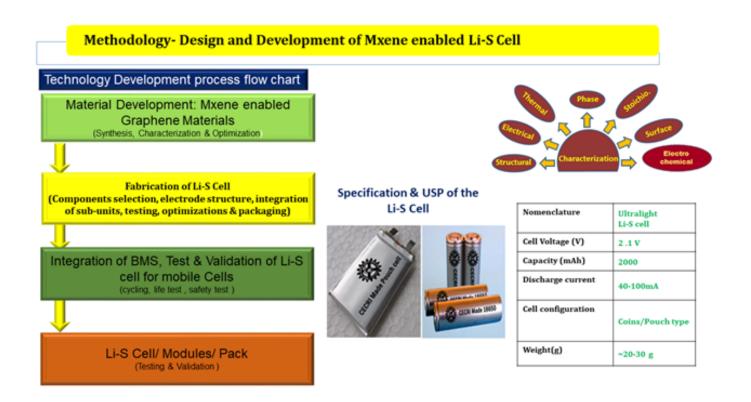
#### Dr. Shantikumar Nair Professor and Director Centre for Nanosciences, Amrita Vishwa Vidyapeetham, AIMS (P.O), Kochi Email - nairshanti@gmail.com

Dr. Shantikumar Nair is the Dean of Research to Amrita Vishwa Vidyapeetham, and also the Director of Centre for Nanosciences, Kochi. Dr. Nair received his Bachelor of Technology degree in Metallurgical Engineering from the Indian Institute of Technology, Bombay, India, in 1976; Master of Science (1978) and Doctor of Engineering Science (1983) degrees in Materials Science and Engineering from Columbia University, New York, USA. He joined the faculty of the Mechanical Engineering Department of the University of Massachusetts, Amherst, MA, USA, in 1985 where he has since taught and conducted research in the area of composite materials. In 2006, he joined Amrita Vishwa Vidyapeetham, India. He heads initiatives in the applications of Nanotechnology to Medicine and Energy areas. Areas of research include nanomedicine, tissue engineering, surface modification of materials, and uses of nanomaterials in photovoltaics, supercapacitors and batteries. In 1986, Dr. Nair received the Presidential Young Investigator Award from President Ronald Reagan for research in composite materials. He is the recipient of the Prestigious National Research Award from the Government of India in 2011 for research in Nanosciences. Dr. Nair received the impressive C N R Rao India Nanosciences Award 2014 for outstanding contributions in Nanotechnology Research and Development in India.

# **26** Design and Development of MXenes enabled Carbon nanostructured materials for Li-S batteries

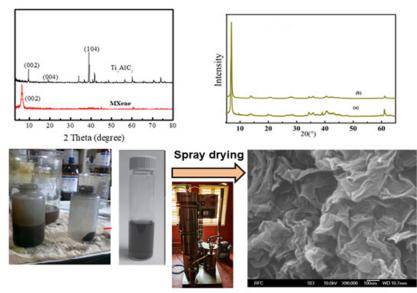
#### Aim

Development of new MXenes enabled Carbon materials as electrode materials for fast charging, high energy Li-S battery by utilize the unique properties of MXenes enabled Graphene nanostructure.



#### **Expected Outcomes & Deliverables**

New Host materials for Sulfur Cathode materials : Sulfur impregnated MXene /Graphene foam	> Light weight, high rated capacity 1200 mAh /g materials
3D conductive network form S/Mxene CNT Composite, S/ Graphene	>high conductivity & Defined pore structured Graphene as conductive and stabilizing framework for the sulfur cathodes
New anode coating	Enhance cycle life • High resistance to corrosion • Reduce electrolyte degradation • Increase volumetric energy
Li-S Cell	High capacity 2.1 V/ 3000-5000 mAh pouch type Li-S cell : Efficiency : 85-95% More than 500 Wh/Kg Energy density Cycle life : target >1000



Crumpled Mxene Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>



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Dr. Kuldeep Singh has received his Ph.D. from the University of Delhi & CSIR-National Physical Laboratory in 2011. He is the recipient of the BRICS Young Scientist award 2016 and the Cooperation of Industry Fellowship award 2011 by the University of Ulsan South Korea. Dr. Singh is an expert in manufacturing of Lithium-ion Cells and process optimization for highperformance batteries with reduced Cost/kWh. Up-scaling of Energy materials, Cell design/ evaluation, Electrochemical testing, Electrode QC, Cell QC, degradation and the associated effect of materials & Li-ion cells/batteries, building business strategies and effective managing teams are his main USPs. His current research interests are rooted in two dimensional (2D) Nanomaterials design and development for Energy storage devices especially Lithium-ion battery, super capacitor for Electric vehicles (EVS) and Electromagnetic interference shielding (EMI). He is leading projects on High energy, fast charging Graphene enabled Lithium-ion cells, multilayer Lithium Sulphur batteries, carbon-based Nanomaterials for structural and energy applications funded by Department of Science, SERB and Industries. He has published more than 40 Research publications in high impact SCI journals having citations of more than 3000 with an h index of 25. He is the editor of two books on energy storage materials & EMI Shielding. Dr. Singh has one patent (India & US) and three more patents on battery technology are in Pending state (India).

# Acknowledgement





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**Department of Science & Technology** 

Vaibhav

#### Cover page photograph:

"Structured Li-ion battery electrode made up of densified Carbon Nanotube cones for high areal loading of active material and efficient electron transport."

**Courtesy:** Dr. Shahab Ahmad, Indian Institute of Technology, Jodhpur.

**Department of Science & Technology** 

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