



Compendium on Materials for Energy Conservation and Storage Platform





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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.



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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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FOREWORD

Advanced materials represent today about 50% of the manufacturing cost of clean energy and are expected to increase to 80% in the near future, according to the Energy Materials Industrial Research Initiative. Thus, a successful transition to clean energy requires the development of new, high-performance, low-cost materials that are resilient, safe for humans and the environment, recyclable, and use abundant elements so that they can be deployed globally. This challenge is not merely an engineering problem; it requires fundamental new scientific advances to design and organize matter from the atomic scale to the systems scale. Identifying the challenges and opportunities associated with the materials discovery, Department of Science and Technology under its clean Energy Research Initiative mounted a thematic research and technology programme on Materials for Energy Conservation and Storage Platform (MECSP). Four MECSP centres set up by Department of Science and Technology, Government of India nucleated at IIT Delhi, IISc Bangalore, NFTDC Hyderabad and IIT Bombay. These platforms will support research and development for entire spectrum of energy conservation and storage technologies from early stage research to technology breakthroughs in materials, systems and scalable technologies to maximise resource use efficiency. These centres will contribute to development of national research network for materials for energy storage. MECSP can be contained in a single facility, housing "well-to-wheel" materials discovery operations. The proposed platform could also quantify uncertainty in materials discovery to help decide whether a particular set of experiments is likely to yield promising results. It could also elevate human creativity away from the details of materials synthesis and calculation, towards a higher-level control of goals-driven design of theoretical and experimental studies, where it is most needed. The report presents portfolio of R&D projects taken up in this initiatives 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.

(Ashutosh Sharma)

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INTRODUCTION

Materials for Energy Conservation and Storage Platform (MECSP) is a theme based initiative to support research and development for the entire spectrum of energy conservation and storage technologies from early stage research to technology breakthroughs in materials, systems and scalable technologies to maximise resource use efficiency. The aim of this call is to create and contribute to a national 'materials for energy network' that includes all the successful centres as well as groups outside the centres in the domains of research, development, and demonstration programmes on energy materials. Energy Storage Platform on Batteries & Energy Storage Platform on Supercapacitors and 2 centres Energy Storage Platform on Hydrogen have been supported for a period of 5 years.

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DST - IIT Delhi Energy Storage Platform on Batteries

Aim

Aim of the ESPOB is to bring together different expertise for the development of redox flow battery, various metal ion-batteries, photo-electrochemical water splitting technologies using earth abundant materials and development of 200W solid oxide fuel cell (SOFC) stack running on natural gas for clean and green energy. The six objectives of the centre are to:

- 1. Develop next generation materials and India-centric scalable energy storage technology
- 2. Material development work on doped-carbonaceous materials
- 3. Develop low cost and efficient hybrid organic-inorganic membrane
- 4. Create human resource pool by training to electrochemical storage technologies
- 5. Network with industry and other institutions (national and international) with complementary skills
- 6. Disseminate knowledge through short courses and workshops to industry and academia

Expected Outcome & Deliverables

- Graphene and modified forms of carbon
- Mixed-metal oxides/ transition metal oxides/ perovskites
- Organic-inorganic hybrid materials.
- Molecular and kinetic simulation and device level modelling

Consortium Members

- 1. Indian Institute of Technology (IIT)Delhi, New Delhi (Lead)
- 2. Indian Institute of Science (IISc) Bengaluru
- 3. Centre for Fuel Cell Technology (CFCT-ARCI), Chennai



- 4. Central Glass and Ceramic Research Institute (CSIR-CGCRI)
- 5. Institute of Minerals and Materials (CSIR-IMMT), Bhubneswar
- 6. Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad

Overseas Partners

- Washington University in St. Louis, USA
- St. Andrews University, St. Andrews, UK

Industry Partner

Hero Electric India



Fig. Flow battery based charging station developed by SERL, Department of Chemical Engineering, IIT Delhi



Fig. Prismatic rechargeable Al–ion Cell, developed at IICT



Fig. A Fuel Cell developed at CFCT Chennai



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Prof. Suddhasatwa Basu, completed his M.S. and Ph.D. from IISc, Bangalore prior to completing B.Tech. in Chemical Engfrom Calcutta University. He is Professor (on lien) at the Chemical Engineering Department, IIT Delhi. At present he is the Director of CSIR-Institute of Minerals & Materials Technology (IMMT), Bhubaneswar. He was earlier Associate Dean (R&D), IIT Delhi and Head of Chemical Engineering Department, IIT Delhi. He has received Herdillia Award for Excellence in Basic Research in Chemical Engineering and A V Rama Rao Research Excellence Award and Indus Foundation award. He is a Fellow of The National Academy of Sciences of India (NASI), Indian Chemical Society. International Association of Advanced Materials, Sweden, Indian National Academy of Engineering, and Royal Society of Chemistry, UK. His current broad area of research consist electrochemical, photo electrochemical water splitting, high and low temperature fuel cells, electrolyser, electrochemical sensor, micro fuel cell, artificial photosynthesis - CO2 reduction, battery and super-capacitor. He has published 250 high impact journals articles with H-index 39. He has authored 10 books and book chapters and patented 5 technological innovations. He is the editor and editorial board member of many journals published by ACS, Springer-Nature and Taylor and Francis.



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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 2014. 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 high impact factor journal articles 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.



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Prof. Aninda Jiban Bhattacharyya, completed his Ph.D. from the Condensed Matter Physics Research Centre, Department of Physics, Jadavpur University, Kolkata. Prior to this, he completed M.Sc.-Physics from Presidency College, Kolkata University. He is a Professor at the Solid State and Structural Chemistry Unit (SSCU), Indian Institute of Science (IISc), Bengaluru. Concurrently, he is the Amrut Mody Chair Professor. His research activities at SSCU, IISc, Bengaluru focuses on frontline phenomena/processes at the interface of physics and His group studies diverse and complex electrochemical phenomena and chemistry. processes in the domain of energy storage, sensing, and biological processes. The strategies adopted extend far beyond the precincts of conventional materials electrochemistry and electrochemical methods. Various sophisticated inhouse and offshore tools are employed to establish the correlation between structure and function. Additionally, the group specializes in the chemical design of novel and multifunctional materials for energy storage and harvesting devices, sensing and actuation. His works have been published in various high impact factor journals of ACS, RSC, Wiley-VCH, Elsevier, ECS and Nature publishing group. He has a total of 140 pulications with a h-index of 32.



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Dr.Vatsala, completed her PhD, from Osmania Uni. in Electrochemistry, started her research carrier as Research Associate in DRDL (DRDO), Hyd. In year 1997. At DRDL generated qualification and acceptance test plans for secondary and reserve batteries for defence application. In 2002 joined CSIR –CECRI, TN as scientist and contributed towards development of alkaline batteries. Moved to IICT Hyd.in 2008. At CSIR –IICT, Hyd., her research focus comprise of development of electrode materials for batteries beyond Lithium. The materials chosen are earth abundant, non-toxic, safe, Mg, Al & Carbon based. Focus is also on development of - non-aqueous, non- flammable, room temperature stable green solvents: lonic liquids as electrolytes. Elaborate studies are in progress on commercialization and scaling up of the polyvalent- ion batteries including safety parameters for practical applications. She is Winner in: DST– Lockeed Martin India Innovation Growth Program – 2015, for development of Mg secondary battery & also Winner in – Visit to USA, Sponsored by DST & Lockeed Martin. She has published 20 research articles in high impact journals, has one patent to her credit.



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Dr Wasim currently working as Senior Scientist in Energy Materials and Devices Division (EMDD) at CSIR-CGCRI, Kolkata. He completed his M.Sc degree in Physical Chemistry from University of Burdwan and received his Ph.D from Jadavpur University, Kolkata in the year 2010 in area of high performance electrode materials for Lithium ion battery (LIBs) technology. After completion his Ph.D, he served as Assistant Manager (R&D) in UNTPL, Indo-US JV limited company dedicatedly working on production of nanostructured electrode materials for LIBs in India. In 2012, he joined as Senior Scientific Officer in Chemistry Division in State Forensic Science Laboratory, Kolkata, Govt. of West Bengal and served till 2020. At Forensic Lab he established a new Management Division in 2017 and was leading a group of 16 scientific personnel for R&D in forensic sciences. He has been honored as guest faculty and National trainer for future safety and failure investigation of high end vehicles (ECUs controlled, EVs, HEVs and autonomous future vehicles) by LNJN-NICFS, MHA, New Delhi. During his stay at battery industry, he got hands-on training in bulk production of electrode materials, fabrication

of 18650 LIB technology and application of LIBs for Mines, solar storage, mobile tower powering energy banks etc. Dr Wasim received MRSI-Young Scientists award (Kolkata Chapter) in 2007 for his contribution in engineered microstructures for high performance battery materials. He published 13 research papers in SCI journals, more than 22 research articles in National/ International conferences on batteries. He patented 6 technology related to synthesis of battery grade electrode materials and paper based ceramic separators. Currently, at CGCRI, he is actively working on developing low cost paper based ceramic separators and Monolithic All Solid State Lithium Batteries (MASSLB). His broad area of research consist of metal-ion batteries, Solid State batteries, synthesis and bulk scale production of engineered battery grade electrode powders, applications of LIB packs and system integration.



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Dr. Mamata Mohapatra received her Ph.D. from Utkal University, Bhubaneswar. She got her post-doctoral experience from University of Waterloo, Canada by availing BOYSCAST fellowship. She joined at Hydro& Electrometallurgy department, CSIR-IMMT in 2006 (October) as Jr.Scientist and has been undertaking research independently on interdisciplinary field of research in aqueous processing of ores and secondaries, synthesis and surface modification of transition metal oxide/ oxalate and carbonate materials for environment and energy application. Currently she is engaged in energy material development through urban mining of sent batteries. She has many contributory well-cited publications in international peer review journals (about 85) in collaborationwithIIT, Kanpur, UtkalUniversity(India), KIIT, MurdochUniversity(Australia), and WATLab (Canada), University of Southern Denmark etc. Her work has received 3485 citations with h index of 27. She has successfully supervised 4 PhD students, 14 M.Sc students, 2 M.Tech students.



DST- IIT Bombay Energy Storage Platform on Hydrogen

Aim

ESPHy is a multi – institutional centre on hydrogen storage systems with IIT Bombay, IIT Guwahati, IIT Kanpur, IIT Tirupati and NIT Rourkela as the partner institutes. The center aims towards developing as a lead focal point in the country in materials and systems research, prototype demonstration, technology development, incubation of innovative ideas, industrial interactions, collaborations, manpower development and information dissemination in the field of hydrogen. There will be industrial and academic collaborations to take the various technologies developed to marketplace. Capacity building and information dissemination in the field of hydrogen will also be the target of the centre.

Goals of the Centre

- National level facility to enable innovations in the area of hydrogen
- To develop the next generation of advanced materials and devices
- Collaborate with National and International level institutions and industries to enable innovations and shared facilities
- Capacity building and educating the next generation of researchers, scientists, and engineers
- Conduct training programs periodically for academia and industry personal and outreach
- Catering to address industrial problems where hydrogen can play major role and provide industrial and societal solutions

 Assist in developing standards, safety protocols associated with hydrogen systems, policy making and act as a point of contact and knowledge centre of the nation in hydrogen

Methodology

There are in all six work packages:

WP 1 : Materials Synthesis and Characterization

WP 2 : Fabrication of metal hydride based fast reaction beds

WP 3 : Testing the performance of various metal hydride based devices

WP 4 : Integration, demonstration an technology transfer of the various metal hydride based systems

WP 5 : Techno-economic and scale up studies on various metal hydride based applications

WP 6 : Human resource development, knowledge dissemination, education and training



Fig. Consortium Members and Major Activities

Expected Outcomes & Deliverables

- Synthesis and Characterization of novel hydrogen storage materials with high hydrogen storage capacity.
- Develop inexpensive materials, which can be produced in larger quantities. Further, the process of synthesis should be amenable to industrial scalability. The materials should be least dependent on critical imports, which implies the restricted use of pure rare-earth metals.
- Facility development for large scale materials synthesis in hundreds of kgs, with 10kg per batch facility being developed.
- Optimization strategies to reduce the number of simulations and modelling experiments required in designing a MH based system while considering heat and mass transfer in such systems.
- Development of a novel reactor containing about 100 kg of MH with improved heat transfer techniques for increasing reaction rates and lowering reaction temperatures and fabrication of metal hydride reactors of different capacities by considering heat and mass transfer aspects.
- Design and development of MH reactors of 5 kW cooling and heating capacity.
- Testing the performances of integrated MH based thermal storage and cooling system and compressor driven MH cooling system at various operating conditions.
- Fabrication and testing of MH reactor for purification of 1 kg hydrogen for industrial application.
- To develop metal hydrides thermal hydrogen compressor to compress hydrogen from 10 bar pressure to 200 bar with a heat source temperature of 150°C.
- For testing the reactor efficacy by, coupling it with fuel cells for power generation and using the reactor for applications like cooling, heating, thermal storage and compressors.
- Investigation of Tech-economic and scale up issues of the developed applications.
- Human resource development, knowledge dissemination, education and training.

Facilities



Thermal evaporation system



Furnace and melting units





Rolling and ball mills





Measurement setups (Static & Dynamic PCI Indigenously developed)





Hydrogen Purification system



Heating and cooling system



TGA-DTA-MS-Hyphenated system

				T Side		
1 Finned tubular canister	4	Tank Canister (filled	7	'Room'	10	Ambientair

	1	finned tubular canister (filled with HT hydride)	4	Tank Canister (filled with LT hydride)	1	'Room' Temp	10	Ambient air blower
	2	Valve to ambient	5	Room to be cooled	8	LT Temp	11	Data Logger
100000000000000000000000000000000000000	3	Hot Air Temp Controller	6	Compressed Air Supply	9	HT Temp	12	Hot Air blower

MH based Air conditioning system



Different reactors with ECT developed for various applications



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Dr. Pratibha Sharma is Professor in the Department of Energy Science and Engineering at Indian Institute of Technology Bombay. Her research interest includes materials for photovoltaic applications, solid state hydrogen storage, materials and systems for hydrogen storage and its utilization.



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Dr. Muthukumar is Professor in the Department of Mechanical Engineering at IIT Guwahati. His area of research includes sorption heating and cooling systems, hydrogen energy storage, metal hydride based thermal machines, coupled heat and mass transfer in porous medium, porous medium combustion, etc. He has published around 280 research articles in various International Journals and conference proceedings and written 8 book chapter. He is having seven national patents for his credit.



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Dr. Anandh is a Professor in the Dept. of MSE at IIT Kanpur. His areas of interest are: Physical Materials Science, Nanomaterials, Quasicrystals, Amorphous Materials, Metastable Materials, Epitaxial Systems, Defects & Interfaces in Materials, Symmetry, Crystallography and hydrogen storage in materials. He is one of the founding members of the Dept. of Sustainable Energy Engineering at IITK, which has hydrogen energy as an important focus area.



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Dr. E. Anil Kumar is currently working as Associate professor in the Department of Mechanical Engineering and Dean Sponsored Research and Consultancy at IIT Tirupati. He is founding Head of Mechanical Engineering Departments IIT Indore and IIT Tirupati. His research interests are measurement of thermodynamic and thermophysical properties of solid-state hydrogen storage materials, Thermal energy storage, carbon dioxide capture and sorption heating and cooling systems.



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Paresh Kale, (Ph.D. from IIT Bombay), currently working as Assistant Professor at Dept. of Electrical engineering at NIT Rourkela. His research interest includes nanomaterials and nanostructures for energy storage and conversion devices – Solar photovoltaics, Hydrogen storage, Battery electrodes, gas sensors. He also works on energy policy, energy economics, cyber-physical energy systems.



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Dr. S. Anbarasu is Asst. Professor in the Department of Mechanical Engineering at National Institute of Technology Rourkela. His research interest includes design and development of solid state hydrogen storage system and its utilization. His other research topics on production of Bio-fuels, and GM type cryo-coolers for low temperature applications.



DST - IISc Energy Storage Platform on Supercapacitors And Power Dense Devices

Aim

The overarching objective of CREST is to develop techno-economically viable electrical energy storage solutions that have the potential to catapult India to a leadership role in energy storage and clean energy technologies through active collaboration and accelerated technology development. In order to achieve the aforementioned, CREST will cater to the following broad aims and objectives:

- Develop national level expertise in energy storage technologies to cater to the immediate energy storage needs of the nation.
- Advance the state-of-the-art in energy storage via the development of new energy storage technologies that have the potential to position India as a leader in energy storage.
- Accelerate energy storage device development through collaborative and synergistic research with active industry interaction.
- Build an advanced national facility, which provides access to academic research.



Fig 1. Broad Research Direction at CREST

Methodology

application-driven The center will primarily focus research for the on development of techno-economically viable electrochemical energy storage solutions with emphasis on high power density storage such as supercapacitors. This will involve development of novel materials and materials' architectures in combination with laboratory prototyping and performance assessment of potential electrochemical energy storage technologies. Technologies identified during this process will be scaled-up for performance demonstration at the battery stack level. With the intent of identifying marketable technologies, our prototype development will also emphasize the assessment of economics of scale. The center also feels the need to share the technical developments during the course of the project for public good. Therefore, biennial conferences that focus on the developments in electrochemical energy storage will be organized. When possible, the center will strive to file patents and transfer technology so as to enable commercialization of the technologies developed at the center. The center will welcome researchers from other academic institutes and industry, which will directly benefit research and lead to the development of skilled work force nationwide.



Fig 2. Broad Research Objectives at CREST

Expected Outcomes & Deliverables

A major objective of the energy storage platform would be to develop national level expertise in energy storage technologies to cater to the immediate energy storage needs of the nation. Our project is expected to identify techno-economically viable energy storage technologies for India's electric grid and electric mobility. In addition, we anticipate advancing the stateof-the-art in energy storage via the development of new energy storage technologies and thereby contribute to positioning India as a leader in energy storage technologies. Continual interaction with industry will be a priority at the center and therefore, we expect that the technologies developed at the center will lead to the creation or advancement of industry and generation of skilled work force. Furthermore, the center could lead to long lasting collaborative research efforts from the investigators of this center with focused research efforts to enable accelerated energy storage technology development within the country. Also, the center could serve as a national center of excellence providing access to industry and academic researchers for carrying out state-of-the-art research and measurements on electrochemical energy storage devices.

Research Areas

Electrochemical Supercapacitors

A major thrust for the center's activities is the development of asymmetric electrochemical supercapacitors with high energy density coupled with the high power densities of supercapacitors. Asymmetric supercapacitors (ASCs) provide higher operating voltage in comparison to symmetric supercapacitors and therefore offer high energy densities while not compromising on power density. Research at the center will focus on ASCs with a novel core-shell

design that could yield single cell potentials of ~2 V. These supercapacitors employ aqueous electrolytes and are therefore expected to offer high current densities. A related research activity concerns the development of Li-ion hybrid ultra- capacitors with a single cell voltage of > 4 V. The high voltages enable high energy and power densities in these ASCs that employ Li-ion electrode materials for the positive electrode and carbon fiber electrodes with nano-architectures as the negative electrode.



Fig 3. Test Set-up for 12.6 V Mn-C Supercapactior

Ion-Intercalation Batteries

The abundance and availability of lithium and cobalt (in LiCoO₂-based Li-ion batteries) could limit widespread adoption of Li-ion batteries. The limited to non-availability of minerals bearing Li and Co within India also necessitates the development of energy storage technologies that utilize elements with high natural abundance within India. Therefore, our research will also involve the development of low cost, high-rate and long cycle Na-ion batteries, development of mixed-ion electrolytes that are necessary for the development of Na/Mg hybrid batteries and also the development of more sustainable organic electrode materials with capacities comparable to state-of-

the-art Li-ion battery electrodes. The use of metallic electrodes such as Mg in Na/Mg batteries will also be researched so as to enable high energy density chemistries that employ metallic negative electrodes.



Fig 4. A Schematic of Na/Mg Hybrid Battery

Redox flow Batteries

Redox flow batteries (RFBs) provide the flexibility to decouple energy and power density of an electrochemical energy storage system. Furthermore, redox flow batteries can be operated at room temperature with a wide operation temperature window. An important storage activity under this theme is the development of large-scale soluble-lead redox flow batteries employing a novel auxiliary electrode concept. In addition, we are embarking on an ambitious research program to develop high voltage (~3 V) non-aqueous redox flow batteries. This project involves a synergetic interdisciplinary effort involving organic molecule synthesis and electrochemical device design. If successful, we would have invented a novel high energy and power density flow battery system with applications in instantly rechargeable electric vehicle batteries.



Fig 5. 3, 5, 7, Cell Stacks Of SLRFB and Preformance of an 8-cell stack of an SLRFB

Chemical Conversion Batteries

Chemical conversion batteries offer very high energy densities and could potentially offer higher power densities when compared to state-of-the-art lithium ion batteries. They are considered as promising alternatives for future energy needs. However, several outstanding challenges such as poor cycle life and dendrite growth on metallic negative electrodes serious limit their commercial development. As part of a futuristic strategic development of energy storage devices, this Center's resources will also be devoted to research and development of designer electrolytes/electrolyte additives for large discharge capacity metal-oxygen batteries; porous carbon networks for high surface area cathodes for metal-oxygen batteries; bi-functional catalysts for advanced Zn-air batteries; and membranes and separators for Li-S and Na-S batteries. Batteries will also be researched so as to enable high energy density chemistries that employ metallic negative electrodes.



Fig 6 .A Schematic of Metal-Oxygen Battery

Investigators



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Naga Phani Aetukuri is an Assistant Professor in the Solid State and Structural Chemistry Unit at the Indian Institute of Science, Bengaluru. Prior to starting at IISc in 2016, he received his doctoral degree from Stanford University in 2013 and worked as a post-doctoral researcher in the Advanced Energy Storage group at IBM Almaden Research Center. His group's research is in the areas of physics of transition metal oxides, electro-catalysis and advanced electrochemical energy storage systems.



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Dr. Satish Patil is a Professor at the Indian Institute of Science (IISc), Bangalore. He did his PhD under the supervision of Prof. Ullrich Scherf at Bergische Universität Wuppertal, Germany on conjugated polymers for blue organic light-emitting diodes. Thereafter, he worked as a Post-doctoral Fellow from 2004-2006 in the group of Prof. Fred Wudl at the University of California, Los Angeles. His academic research interests include synthesis of conjugated polymers and oligomers with novel properties and studying their characteristics working at the interface of chemistry, physics and materials engineering.



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DST - NFTDC Centre For Materials & Energy Storage Platform on Hydrogen

Aim

- Conduct state of art TRL 3-7 translational R & D in Materials to H₂ based energy devices in the area of SOFC, H₂ Storage and Metal Hydride sorption cooling
- Conduct Research in development of novel materials as composites, graded materials, mixtures, materials + catalysts around the well – proven base material to meet the figure of merit for SOFC, H₂ storage and Metal – Hydride sorption cooling;
- To develop cost effective processes for synthesis, deposition, thermal treatment, thermo-mechanical processes, joining, precision manufacturing and assembly for enabling both materials development and their scale – up on one hand and materials to products manufacture on the other;
- To develop innovative designs and design for manufacture (DFM & DFA) of energy devices and conduct extensive simulation and modelling to distil high performance design configurations;
- Design, develop and fabricate cost effective process equipments for materials synthesis and manufacture of devices
- To render the device designs in a process product integration and optimization paradigm in TRL 4-6 translation to manufacture prototypes;
- To fill gaps in front end (BOS) and back end (fuel) and undertake larger system level development and eventually graduate to TRL -7 pilot production of devices.
- Develop functional test beds and conduct long duration testing of the device; integrate the device in field level applications;

- System level modeling and simulation to iterate the designs to optimize the performance parameters of efficiency, cycle life, ease of manufacture and cost metrics;
- Upgrade pilot plants and establish pilot plant for scale up of advanced materials such as RE oxides, catalysts, RE alloys in NFTDC to ensure supply chain based on indigenous RE materials;
- Study techno economics for feasibility of large scale product manufacture and market acceptance;
- To conduct focused workshops on SOFC, H₂ storage and Hydride Sorption cooling on periodic basis.
- To train the next generation researchers in the area of SOFC, H₂ storage and Hydride Sorption and develop system level thinking and engineering
- To interact with energy companies in India and abroad to translate product to business

Methodology

Work Package – 1: Reformation, CHP and BOS in SOFC Systems. (Target: Integrated Device for demonstration 1kW) Implementing Institutions: NFTDC + IISc + IIT BBSR

(a) Reformation System based on CNG Input Feed, Utilization of exhaust heat & H₂ Recovery To produce hydrogen from hydrocarbons, Steam - Methane Reformation of natural gas (methane) is the most common method. In the Reformer, methane and steam are reacted together over a Ni impregnated alumina catalyst at a temperature of 600-800 0C and 3-5bar pressure. The reaction product is Syn-Gas which is a mixture of Hydrogen and Carbon Monoxide. For bulk production of hydrogen, CO has to

be removed from Syngas via Water gas shift reaction, a two-stage process and endothermic in nature wherein CO can be converted to CO_2 . An alternative process for removal of CO as CO_2 is via Tail Gas Oxidation over Copper Oxide Catalyst which is a single stage process normally carried out around 45°C. CO_2 is them scrubbed out in an absorption column. Hydrogen of 95- 99% purity can be achieved in a combination of methane reformation and tail gas oxidation routes together with CO_2 absorber which is being adopted in this project.

A reformation unit comprising of above three sub – systems, namely methane – steam reformer, TGO and absorber for production of in – situ H_2 from CNG feed will be set up to study the mass flow rates, energy balance and conversion efficiencies to H_2 . This system will be then miniaturized in to multiple micro – reactors to obtain a robust front end in – situ H_2 production unit as a product for ITSOFC. Trials of this reformation unit will be first conducted with fuel cell test bed (0.5KW) before for optimization of overall utilization of H_2 in terms of power produced, feedback of H_2 for heat generation vis a vis H_2O scrubbing to recover H_2 for feed minimization.

(b) Optimization of SS interconnects with gas channels for better distribution and utilization of fuel and weight (thickness) reduction of interconnects.

The first and foremost factor to be optimized in the interconnects is the routing of gas channels so as to not obtain dead zones and to enhance fuel utilization. Modelling and simulation experiments together with thermography using hot air/Ar/H₂ gas for study of flow channels in a single IC set–up at operational temperatures of IT SOFC will give first hand quantitative information on design parameters vis a vis H₂ feed from channels to Anode / Cathode porous metal substrates at operational temperatures of $60^{\circ} - 70^{\circ}$ C.

(c) Materials to Cells & Cells to Stack

NFTDC developed materials as in CGO, YSZ, LSCF and also scaled up the process to 10 – 20 kg batch levels. Furthermore, the deposition process methods such as ink jet printing, plasma spray (solution) and magnetron sputtering have been optimized.

(d) Long duration testing & component degradation analysis

NFTDC will be conducted to optimize the cell performance vis a vis deposition parameters and stack related parameters as flow rates, distribution with the existing SOFC bed.

(e) System Level Modeling Simulation

Combined reformation + SOFC stack system has to be modelled for Heat transfer as well as CFD so as to understand fuel utilization, optimization of gas channels, identification of hot spots, flow parameter optimization. In addition, thermodynamic efficiency computation for various scenarios has to be investigated so as to maximize CHP efficiency.

(f) Incorporation of on board thin film sensors for T and H_2 gas sensing.

Thin film temperature thermocouple (TFTC) based on Pt – PtRh of less than 30 micron thickness has been developed in a companion project. This TFTC will be embedded in the IT SOFC on bipolar plates to not only study the temperature uniformity and health monitoring of individual cells. Gas sensors (H_2 sensors) in gas lines will also be incorporated in the system for safety measure.

(g) Balance of Systems (BOS)

BOS pertains to storage options in a battery, conversion of DC to DC and DC to AC

as per load requirements. Furthermore, control of Stack along with reformation units needs safety sensors to be monitored with HUI with appropriate inter-locks.

Work Package – 2: Magnesium – Carbon based H₂ Storage Systems Development Implementing Institutions: NFTDC + IITM + Sri Chitra Trunal

(a) Development of Process and Manufacturing equipment for Graphene production

The design of the process equipment will be undertaken as we have a 2.54GHz MW and 6kW power microwave system. The innovation is in the design and development of the applicator with provision for creation of mist of organic liquids containing carbon which are to be experimented in low pressure argon plasma. Membrane filtration followed by sonication is the method followed to separate the graphene products. The process is very fast as the reaction times of the order of seconds. This process is scalable in terms of number of nozzles, length of MW – plasma zone created and is also amenable for insertion of other solids such as powders of metals or oxides in concentric nozzles or separately.

(b) Materials Development and Scale – up

Mg + Carbon and Graphene materials development for solid State Hydrogen Storage; From the above paragraphs, it is clear that in the project we have to concentrate on only two materials, namely Mg + Carbon as ENG/Graphene. So far, up to 5% ENG has been extensively studied by NFTDC and other research groups across the world. We have two extremes, namely 100% MgH₂ and 100% carbon based systems. It is anticipated that Mg + additives + Graphene combination has the potential to give desorption temperatures around 200°C and also possess more than 5 Wt.% gravimetric storage capacity. The additives to be studied to be are TiFe, Zr, LaNi5 in a nano-material sizes and in terms of relative proportions. In a PCT set – up H₂ storage capacity will be experimentally investigated.

(c)System Level Modeling and Simulation for device development

IITM team and Chitra Trunal College of Engineering shall undertake system level modeling for device development. Based on the simulated models, a storage device will be developed and fabricated. Device level testing particularly for its desorption characteristics will be done in the test bed in NFTDC.

Work Package – 3: Hydride Sorption Cooling based on waste heat/ solar thermal (CSH) >> Materials, Design and Device DevelopmentImplementing Institutions: NFTDC + IITM + Sri Chitra Tirunal.

(a) Process Equipment Design and Fabrication for manufacture of La-Ni-X materials

Vacuum melting following by centrifugal powder preparation in a nozzle jet is a potential one step process for manufacture of La-Ni- X powders. NFTDC has developed many vacuum melting and casting apparatus and equipments. In this project, a dedicated centrifugal powder preparation equipment of 1- 1.5 kg will be designed and fabricated. Rapid heating to 150° C, high rpm rotation and ejection of melt through ceramic nozzles and quenching on water cooled copper sinks are the salient attributes. This equipment development reduces the cost of procurement of atomization kind of apparatus at high costs.

(b) Manufacturing Methodology:

Fabrication of sorption cooling device requires (i) materials synthesis & its PCT characterization; (ii) fabrication of capillaries, meshes and beds, (iii) hermetic sealing; (iv) incorporation of sensors and fast action valves; (v) waste heat /solar CSH integration for the HT end; (vi) heat rejection systems (exothermic heat during absorption of hydride to the ambient) and its operations (vii) instrumentation and control;

(c) Engineering design of the twin hydride system

It is to be optimized so as to achieve the best COP, time for T drop from 40°C to 20° C for a given cooling load and volume. Various bed designs such as Capillary Bundle Tube Reactor (CBTR), Metal Foam Tube Reactor (MFTR), multi stage hydrides and artery-vein biomimetic design have been studied. Biomimetic design pioneered by NFTDC in the earlier project has been found to be the most efficient of competing designs. Design for Manufacture & Assembly (DFM & DFA) is to be front – loaded in the design paradigm of the device. Instrumentation & control systems for operation of cycle and HUI.

(d) Testing:

A functional test bed of 1m3 volume, to be cooled, will be set up and all the performance parameters will be evaluated over 1000s of cycles.

Expected Outcomes & Deliverables

- Cost effective development of 1 1.5 mm thick Ni foam and area 100 x 100 mm and pro cess scale up to produce 100s numbers of such foams. (currently Ni foams are very expensive and are imported); SS powder based porous supports and scale up
- Repeated in-house operations to produce anode (NiO), electrolyte (GDC), and LSCF (Cathode) and YSZ (interlayer) at 5 kg level.
- Plasma Gun modification to enable both powder and solution spray.
- Repeated production of cells (50mm and 80/100 mm) with all layers
- Simulation of interconnect passages for efficient gas utilization

- Achievement of Stack level sealing (leak tightness against thermal cycling)
- Stack Performance: OCV, Current and wattage at $75^{\circ} 90^{\circ}$ C with H₂ gas
- Reformation Kit: BioSyn Gas (IISc) and CNG (NFTDC)
- System integration with reformation kits
- Stack Performance: OCV, Current and wattage at 75^o 90^oC with reformed Gas
- Long Duration Testing: 100 Cycles and 1000 Cycles
- Degradation analysis after 100 Cycles and 1000 Cycles.

IISc, Bangalore:

- Performance characterization of SOFC with range of H₂-CO mixtures benchmarked against baseline Hydrogen fuelled operation
- Carbon boundary for dry mixture and relative humidity levels required for carbon deposition free operation
- Mini Methane reformer setup
- 1. Catalytic reforming A mini Methane reformer to generate syngas designed to operate at small capacities (LPM level) and at low pressure conditions.
- Plasma based reforming A non-thermal plasma based reformer to generate syngas under both dry and humidified conditions operating at near ambient conditions
- 3. A custom designed burner for handling the tail gas, especially at low CO levels.



Reformation Equipment at NFTDC – Shipped to IISc Bangalore



Fuel cell testing lab at NFTDC



SOFC fuel cell stack



Plasma Lab at NFTDC for spray coating for Fuel Cells



Air-Plasma Gun Prototype Design



Air-Plasma Gun parts – Design



Air-Plasma Gun parts Fabrication & Assembly



Ink jet Printer



Nozzle



SOFC Test Station – IISc



Plasma Methane Reforming Schematic



Carbon boundary for SOFC

Early MS-SOFC development – IIT Bhubaneswar:

- Preliminary studies of flame spray deposition of zirconia-based electrolyte onto pre-sintered austenitic stainless steel support (power density: 115 mW.cm-2 at 750°C) were carried out.
- Pre-fabricated tubular NiCrAlY and planar CrFe₅Y2O₃ supports were coated with plasma sprayed zirconia electrolytes. Power densities approaching 1 Wcm-2 were achieved at 900°C.

The following are the advantages of planar design:

- Fabrication flexibility
- Low cost
- Ease of flow arrangements
- Higher power density



SOFC Performance With CO-H₂ Mixture



The choice of metal support should be such that the coefficient of thermal expansion of substrate should match with electrolyte to enable thermal cycling, low oxidation rate and has low cost.

Surface oxidation studies were carried out on SS316 – substrate and it was observed that with an increase in time, surface oxidation of SS316 increases as shown in EDS mapping.



Electron Image



Electron Image 1



Electron Image 1



EDS mapping of surface oxidation of SS316 substrate

Magnesium – Carbon based H₂ Storage Systems Development

- Design and Fabrication of Microwave based Graphene Production Apparatus;
- Rendering of PCT DSC apparatus
- Production of Mg coated with Graphene (100 gm)
- Testing of absorption and desorption (10 cycles); Material should not degrade in PCT -DSC
- Modeling & Simulation of storage device
- Design of hydrogen storage reactor considering design for manufacturing and design for assembly
- Optimizing the reactor for better performance with minimal weight and cost
- Prototype of Device and Testing



6 kW microwave set up for producing Graphene - NFTDC



Reactor design at IITM



Study on effect of coolant velocity on wt% of H2 in the reactor



Compendium MECSP 2017



Concentration contours at t=300 s for fin lengths L=4, 8, 12 and 16mm

Hydride Sorption Cooling based on waste heat/ solar thermal (CSH) >> Materials, Design and Device Development

- Successful Design and Fabrication of Centrifugal Powder Production Apparatus
- Synthesis of La-Ni-X powders (one kg per run)
- Testing of materials in PCT DSC
- Simulation of biomimetic design
- Engineering Design and Design for manufacturing
- Prototype fabrication of twin reactor system
- Testing with applicator (cabin and automobile)



Design of prototype for powder production – Vacuum Centrifugal Caster



Fabricated Vacuum Centrifugal Caster at NFTDC



Heating trials



Casted alloy from Vacuum Centrifugal Caster



PCT apparatus developed at NFTDC – Supplied to IIT M



PCT Software developed at NFTDC



Numerical Study of Metal Hydride Storage Device Embedded with Phase Change Material



Numerical Study of Metal Hydride Storage Device Embedded with Phase Change Material – Sri Chitra Trunal



Temperature vs. time profile for metal hydride and phase change material – Sri Chitra Trunal

Research Areas -

Work Package – 1:

- (a) SOFC materials Bio syngas / Fuel reformation
- (b) Device design BOS
- (c) Experimental and numerical investigation of SOFC
- (d) Reforming of methane to generate syngas
- (e) Burner design for tail gas utilization

Work Package – 2:

- (a) Magnesium based materials + graphene
- (b) Process equipments (PCT DSC)
- (c) Simulation and modeling
- (d) Device design, fabrication and testing

Work Package – 3:

- (a) Study on La-Ni-X-Y systems for sorption cooling
- (b) Simulation and modeling
- (c) Device design, fabrication and testing



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Dr K Balasubramanian, graduated from the Indian Institute of Technology (IIT), Kanpur, India with a B.Tech in Metallurgical Engineering in 1982. He proceeded to the School of Materials Science and Engineering at McMaster University, Canada to pursue a direct PhD on being awarded the ALCAN fellowship. His research interests in the last 25 years span into many end to end Technologies encompassing materials, processes and application engineering in a systems approach. Dr. Balasubramanian was the architect in conceiving the (i) Centre for Engineering Design & Manufacturing, (ii) Centre for Biomedical Devices dedicated to implants and reconstructive surgery, (iii) an advanced centre for motors, (iv) Centre for Materials and Energy Devices, (v) Centre of Excellence in xEV Drives under National Mission on Electric Mobility thus creating a true multidisciplinary laboratory that is well geared to take up end to end technology solutions graduating NFTDC from materials Lab to a Systems Level Technology Centre. He has published over 100 papers in international journals; holds 7 patents and has guided many for PhD in materials, processes, pattern recognition, knowledge management and reconstructive surgery which are of interdisciplinary nature. He has won many awards and laurels for his contribution to Science and Technology.



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Cover page photograph:

"Lithium dendrites in High Voltage Lithium metal-based Solid State Li-ion batteries"

Courtesy : Dr. Naga Phani Aetukuri, Indian Institute of Science (IISc), Bengaluru, India

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