

विज्ञान एवं प्रौद्योगिकी विभाग DEPARTMENT OF **SCIENCE & TECHNOLOGY**



DST-IIT Hyderabad Integrated Clean Energy Material Acceleration Platform on Bio-energy and Hydrogen

A Consortium on Green Hydrogen: Evolution to Revolution



















A collaborative AI/ML enabled accelerated technology development platform for sustainable hydrogen generation and storage from waste biomass.

QUOTES



The Integrated Clean Energy Material Acceleration Platform (MAPs) would bring best minds together and is expected to lead to research and technology outputs of immense value for clean energy driven growth. MAPs would also accelerate the pace of material discovery up to 10 times faster in clean energy domain for cost effective, reliable and robust solutions.

Dr. Jitendra Singh

Union Minister for Science & Technology, Earth Sciences, Environment, Forests and Climate Change-Government of India



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> **Dr. Srivari Chandrasekhar** Secretary, Department of Science & Technology Ministry of Science and Technology - Government of India



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> Dr. Anita Gupta Head, TMD (Energy, Water & all Others), DST Ministry of Science and Technology - Government of India



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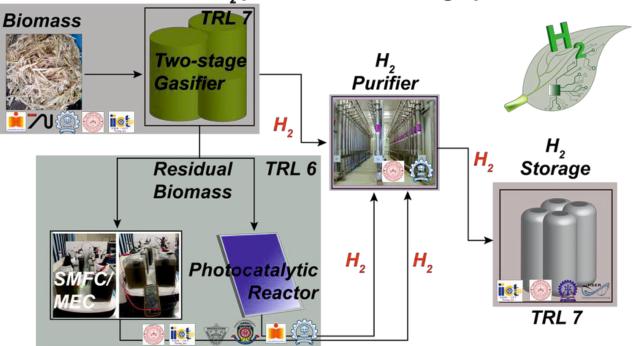
> **Dr. Ranjith Krishna Pai** Scientist, TMD (Energy, Water & all Others), DST Ministry of Science and Technology - Government of India

ABOUT THECONSORTIUM

There is increased awareness that concerted steps need to be taken to reduce CO_2 emissions in order to limit the ongoing global warming to levels less than 1.5°C above preindustrial levels to avoid potentially damaging economic and health impacts. Various countries, including India have pledged to Nationally Determined Contributions to reduce the CO_2 emission intensity of energy, production and transportation sectors. Hydrogen from sustainable sources is increasingly being seen as an important component towards a zero carbon pathway as it can be used to decarbonize hard to abate sectors and balance the intermittency issues of traditional renewable energy sources. Hydrogen production and storage from waste agro– biomass has enormous potential as it can simultaneously generate hydrogen with no net CO_2 emissions (unlike traditional hydrogen production technology) and provide a means to effectively add value to agro–forestry waste resources.

The DST ICMAP Bioenergy and Hydrogen consortium aims to accelerate the development of ultra–efficient commercially viable biomass and waste–water to hydrogen conversion and storage systems through accelerated discovery of novel catalysts, novel storage systems and materials, and optimized plant condition designs enabled by state–of–the–art Artificial Intelligence and Machine Learning Platforms.

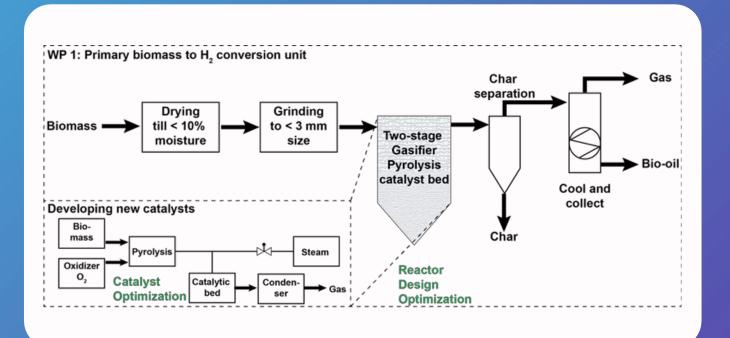
The project envisages a multi–stage H_2 production where, initially H_2 will be generated through a two–stage catalytic steam gasification of dried biomass. The waste–water and tar byproducts of biomass gasification will be fed through a microbial electrolytic and microbial fuel cell as well as a photocatalytic reactor for further generation of Hydrogen. Several optimized versions of adsorption and absorption based Hydrogen storage systems will also be developed to significantly enhance the present technical capabilities of volumetric and gravitimetric hydrogen storage. Emphasis will be on using low cost materials, high conversion and storage efficiency and scalable synthesis.



Biomass-derived H, production & storage pilot: IC-MAP

Work Package 1 Hydrogen through biomass gasification.

A two-stage gasifier will be developed on a pilot-scale for the initial treatment of biomass for H₂ production. Here, the catalytic bed will include newly designed catalytic materials for improved biomass to H₂ conversion. Work Group 1 intends to demonstrate a Hydrogen yield of 100 gm/kg biomass at the bench scale and 75 gm/kg of biomass at the pilot scale with thermally and chemically stable catalysts. This will be approximately twice the yields demonstrated at the pilot scale for steam-based Biomass gasifiers as per available literature. Al enabled catalyst material design and gasifier design optimization through detailed modelling will be used to achieve the goals. Rice husk, stubble and sugarcane bagasse will be used as input biomass. The pilot scale biomass gasifier will be constructed and will be able to handle 25 kg of biomass per day.

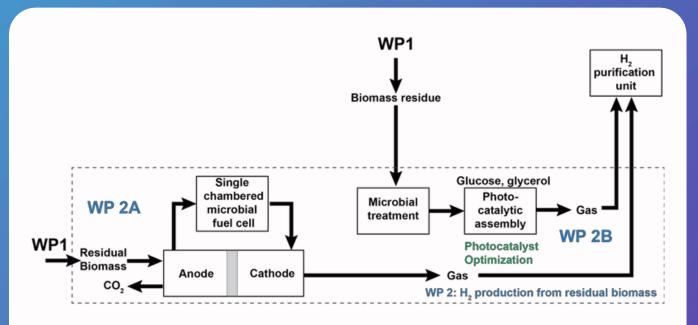


Work Package 2A Hydrogen through microbial SMFC-MEC cell.

The biomass residue developed in WP1 will be used as the ingredient in WP2 for further extraction of H $_2$ via two distinct routes. In WP2A, an assembly of SMFC/MEC will be employed for biohybrid system-driven H $_2$ production. The main goal is developing an energy input free SMFC-MEC system for pure H $_2$ production and bioelectroremediation of liquified biomass derived from WP1 and wastewater. Al/ML enabled acceleration platform will be used to develop and deploy novel cost-effective and environmentally sustainable materials with suitable topology to enhance microbial growth, having higher resistance to pH variations and better electrical properties for use in this optimized SMFC/MEC system.

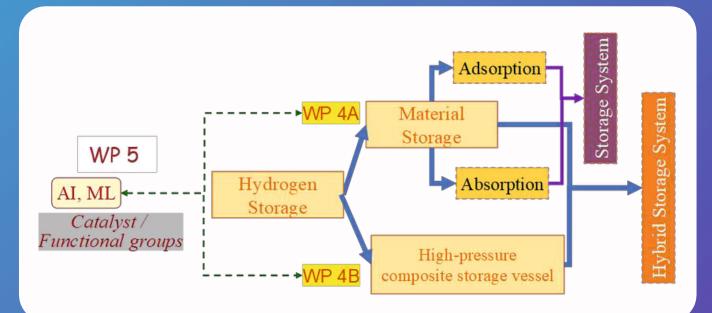
Work Package 2B Hydrogen through photo-catalysis.

In WP 2B, the biomass waste coming from WP 1 and WP 2A is sent to the photocatalyst panels that produce sunlight-driven H_2 by just using sunlight, without the need of any electrical bias. To further advance the efficiency of H_2 generation at scale, rational insights on the photocatalyst design and large-area panel fabrication will be obtained through AI/ML enabled material discovery acceleration platform.



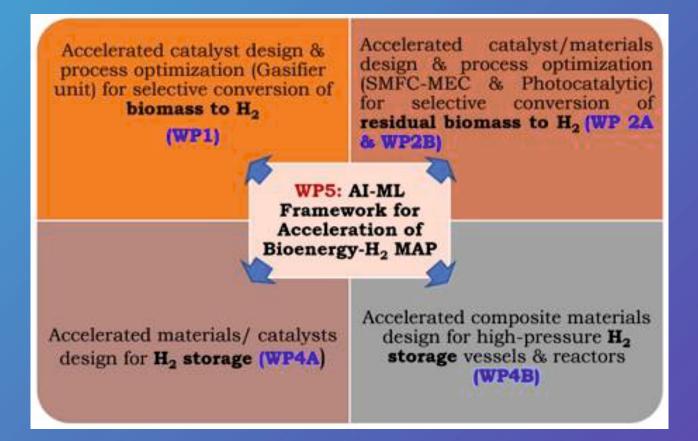
Work Package4 Hydrogen storage in materials and cylinders.

The objective of the hydrogen storage subgroup is to come up with a prototype of a storage unit that has the capability of storing hydrogen in both material form (WP4A) as well as cylinder form(WP4B). The material-based prototype would have a very high gravimetric capacity, good kinetics, would work at low pressures and temperature conditions which have not been hitherto achieved. Additionally, the material would be cost-effective such that it is amenable to scalable synthesis. Both adsorption and absorption based materials will be investigated. A device would be fabricated to incorporate the material developed. The high-pressure storage system will be state-of-theart, which is capable of withstanding very high pressures (700 bar). The material, the micro-structure and fabrication technique for the same will be developed a part of the project. Virtual prototype of any size and shape and working pressure will be designed, fabricated, and tested using the characteristics and property of materials developed. Virtual testing for the preliminary tests will record the response of the device in situations of accidents due to fire or burst. The results of virtual testing will be used to reform the device hereby reducing the risks of sudden failures in emergency situations.



Work Package 5 **AI/ML MAP Platform Development.**

WP5 is tasked with the development of the AI/ML enabled Material Acceleration Platform. The tasks will include database and literature search for process conditions and catalysts/photocatalysts/ materials for biomass gasification, SMFC-MEC, and photocatalytic conversion of biomass and residual biomass to H_2 , datamining of materials/catalysts for H_2 storage, dopant data search for carbon based high surface area adsorption system, Metal alloy-based hybrid absorption system, and Composite materials design and fabrication conditions data search for high-pressure storage vessels. The project tasks also include formulation and development of predictive ML models for existing catalysts/ materials, H₂ storage materials/catalysts & composite high-pressure storage vessels for understanding structural Icomposition-property relationships.





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DST-IIT Kanpur Integrated Clean Energy Materials Acceleration Platform on Materials

A consortium for the Development of Materials and Devices for Energy Harvesting and Conservation Technologies



























QUOTES



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DST-IIT Kanpur Integrated Clean Energy Materials Acceleration Platform on Materials center brings together our strengths in solid-state physics, computational materials science, materials synthesis and characterization, device fabrication, machine learning, automation and reliability evaluation to help accelerate the development of techno-commercially viable clean energy technologies. Prof. Kanwar Singh Nalwa

Center Head & Administrative PI Indian Institute of Technology Kanpur



The primary research emphasis at the center is the development of energy harvesting and conservation materials possessing excellent functional performance and ambient stability. DST-IIT Kanpur center could enable the fast-paced translation and subsequent commercialization of perovskite solar cells, solar thermal receivers, smart windows and thermal insulating tiles. Prof. Birabar Ranjit Kumar Nanda

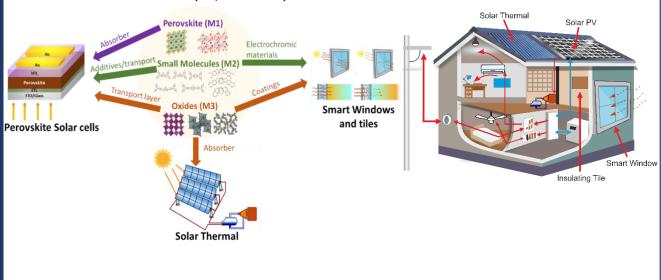
Center Lead PI

Indian Institute of Technology Madras

PREAMBLE

As renewable energy production is gaining the spotlight, silicon-based solar photovoltaics are receiving increasing attention as a potentially pervasive approach to sustainable energy generation. However, silicon-based solar cells fabrication is a very high energy-intensive and complex The perovskite holds the upper hand over technology, which makes the solar modules costly. silicon technology for its solution-processed approach resulting in efficiency comparable to silicon cells while using cost effective and facile synthesis and fabrication technology. The ambient stability of the perovskite is the foremost hurdle for the commercialization and new strategies will be developed at the DST-IIT Kanpur Integrated Clean Energy Materials Acceleration Platform on Materials center to enhance the stability and performance towards the commercialization of perovskite-based solar cells. India particularly has a high potential to integrate solar energy technology with the smart energy management system which will lead to reduced utilization of conventional energy. Therefore, one of the objectives of the center is to design and develop performance materials for solar thermal systems, and thermal tiles and smart windows for energyefficient buildings. Such cost-effective and marketable building-integrable technology can leverage the entry of Indian industries into the respective market in line with the 'Make in India', 'Innovate in India' and 'Atmanirbhar Bharat' initiatives of the central government.

The successful execution at DST-IIT Kanpur Integrated Clean Energy Materials Acceleration Platform on Materials center is envisaged to deliver critical information on the design and development of new and high-performance materials, solar cells, prototype coatings, smart windows, tiles and solar thermal components and a catalogue of potent materials and device components will be generated over the tenure of the project. Our team comprising of researchers from the IITs (Kanpur, Roorkee, Madras, Guwahati and Hyderabad), CSIR (IICT and NIIST), IIITDM, IISER Thiruvananthapuram, NIT Tiruchirappalli and ARCI Hyderabad, brings in expertise from various facets of energy harvesting and conservation including photovoltaics, solar thermal storage, materials synthesis and characterization, automation, computational materials science and machine learning into a unified synergistic working group. The proposed deliverables of the center can potentially be integrated with numerous clean energy technologies that can be immediately employed by industry, making it versatile in terms of national and global acceptance.

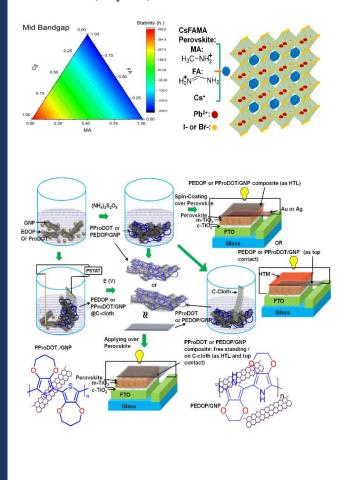


Materials Modules (M1, M2 and M3)

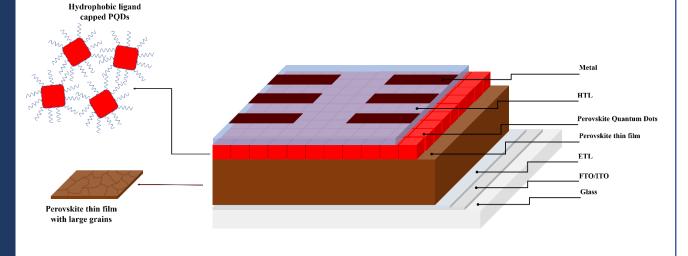
RESEARCH AREAS

Perovskite Solar Cells

As far as the energy harvesting is concerned, the halides with perovskite architecture have emerged as the most promising photovoltaic materials which are cheap, scalable and solution processible. Even though power conversion efficiency (PCE) greater than 25% is achieved, the photo, thermal and moisture stability of these materials is far lower (less than 2 years) compared to other commercial PV technologies such as silicon PV (30 years).

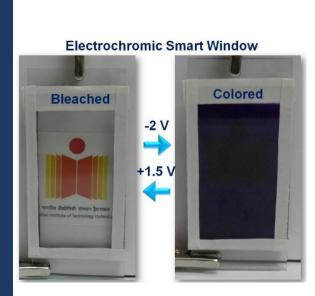


The primary objective of the DST-IIT Kanpur Integrated Clean Energy Materials Acceleration Platform on Materials center will be to design materials for energy harvesting by employing quantum and classical mechanics-enabled atomistic simulations and AI&ML algorithms. We will scan a large compositional and configurational space for predicting new materials for low-cost clean energy materials and for efficient energy harnessing. We will also employ compositional engineering of the perovskite material to improve both efficiency and the stability of the PSC. Small molecule and polymer-based additives will be incorporated to improve perovskite crystallization, passivation of defects in the bulk and/or at the surface, and can also tune the energetics and the structure of the interface for increased ambient stability. We will also work towards the development of low-cost, thermally and chemically robust transport materials, both hole and electron transport layers based on metal oxides to improve the thermal and photostability of the resulting solar cells. Automated advanced optical and electrical characterization and analysis of the perovskite solar cells will be performed to study and elucidate degradation mechanism. the materials The materials and device characterization data will be fed AI/ML algorithm into to predict environmentally robust compositions, that will be synthesized using automated and roboticized processing flow.



Solar Thermal





Smart Windows

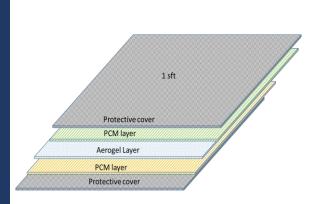
RESEARCH AREAS

Solar receivers/collectors play an essential role in solar thermal-based hot water heating and cooling systems for buildings, steam generation for various industrial applications, and power production. Solar thermal energy is extensively used in industrial and domestic applications like solar drying operation, space heating, cooling, water heating, desalting of water, etc., by nonconcentrated and concentrated solar thermal (CST) systems. The solar receiver tube is one of the critical components in solar thermal technology. The evacuated tube solar collector is the most extensively used solar thermal collector in the market. The development of novel materials with low cost and high solar absorptance is more critical for economic and high-performance solar energy harvesting and thermal energy storage systems. Transition metalbased spinel is a suitable candidate and are typically used for solar absorber material due to the presence of partially filled d-orbitals, which allows for excellent absorption of solar radiation and is tuned to get a spectral selective nature by a suitable combination of two or three transition metal oxides. At the first stage synthesis of nano spinel and low refractive materials (MgF₂/ SiO_2) will be performed for coating development from lab to prototype receiver tube (1m). Moving we will focus spinel-based forward on nanocomposite PCM from lab to 1 kWh prototype. Further, design and fabrication of solar receiver tubes and thermal storage system Integration and validation by using center's facility.

The exponentially increasing demand for energy in the domestic sector may be mitigated to a large extent by efficiently modulating the indoor temperature and light. A reliable smart window technology can lead to efficient utilization of energy by modulating indoor cooling and lighting and together with import substitution, this technology will directly result in profound national, industrial and societal impact. Netpositive energy buildings are an integral part of a designed smart city and smart windows form inevitable components of such buildings. At DST-IIT Kanpur center we will be synthesizing a wide range of novel viologens confirming their applicability to smart windows by characterizing them in terms of their electro-optical properties kinetics, optical modulation, (switching reversibility, coloration efficiency) and their operational and shelf stability in the form of small area devices. The best performing electrochromic materials and electrolytes will be scaled up.

RESEARCH AREAS

Thermo-Regulating Tiles



Target to achieve

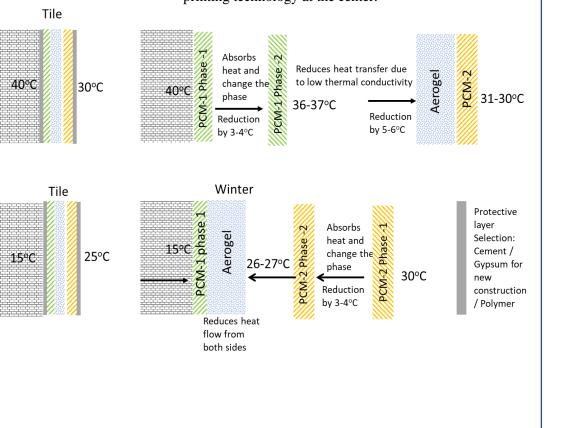
Wall

Wall

60°C

10°C

Thermal insulation to the buildings for reducing the indoor ambient temperature in summer and keeping the indoor space warm during winter is the most desired product, which can reduce the electricity load required for air conditioning. The products available in the market related to this domain are thermal insulation paints for walls and roofs, plaster, bricks, etc. Presently, thermal insulation is generally achieved by adding hollow glass microspheres to the matrix such as paint or putty. In order to achieve the optimum temperature inside the building, DST-IIT Kanpur Integrated Clean Energy Materials Acceleration Platform on Materials center will use a high enthalpy and low-cost solid-state (SS) shape stabilised phase change material along with the existing aerogel technology for producing an effective thermo-regulating tiles. SS shape stabilised phase change materials for thermal energy storage have received increasing interest because of their high energy-storage density and inherent advantages over solid-liquid counterparts (e.g., leakage free, no need for encapsulation, less phase segregation and smaller volume variation). The novelty of this investigation is the development of thermos-regulating tiles with a PCM (SS/Shape stabilised) and Aerogel powder that will be fabricated with the help of 3-D printing technology at the center.





External Quantum Efficiency

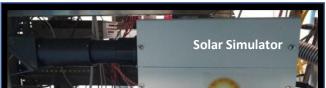




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FluoTime 300 Lifetime Spectrometer







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DST-IISER Thiruvananthapuram Integrated Clean Energy Material Acceleration Platform on Storage

A Consortium for the Development of Solid-State Battery Technology

An initiative to accelerate the development of solid-state battery technology using machine learning (ML) and artificial intelligence (AI) through automated processes.



















PREAMBLE

The intermittent nature of renewable energy sources and increased focus on Li-ion batteries as the power source in electric vehicles has pushed the development of batteries with significantly lesser charging time, higher energy density, and better safety. The replacement of conventional liquid electrolytes with solid lithium-ion conducting membrane as the electrolyte promises all-solid-state batteries (ASSB) with improved safety due to the absence of flammable organic solvents. Apart from enhanced thermal stability, ASSBs are expected to be better in terms of energy density as it allows the use of high specific capacity lithium metal as the anode. Further, in all-solid-state batteries, various cells can be stacked together in a module without casing for the individual cell, which results in a simpler fabrication process and additional improvement in energy density at the module level.

We intend to automate the characterization of identified cathode & electrolyte materials for room temperature conductivity, ionic transference number, and impedance of assembled cells in a wide frequency range. Further, the fabrication of all-solid-state cells using various techniques such as electrospinning, curtain coating, and 3-D binder jet printing technique is planned for upscaling the ASSB towards commercialization. Machine learning (ML) and artificial intelligence (AI) methods have been developed that can substantially accelerate first-principles modelling. Based on the modelling and theoretical predictions, the experimentalists will synthesize and characterize identified compositions. We will utilize automated 3D Binder Jet Printing and large-scale curtain coating techniques to fabricate solid-state batteries.

QUOTES



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IISER TVM, nestled in the beautiful Western Ghats of 'God's own country', is reputed for high-quality education through research engagement in the most tranquil atmosphere. With world-class infrastructure, enviable facilities and scientists of exemplary calibre, IISERs have emerged as sought-after destinations for inquisitive and passionate young minds to conduct research on emerging areas. IISER TVM wholeheartedly welcomes the IC-MAP STORAGE centre to the campus. We are certain that the new addition will pave way for innovations in solid-state battery research. **Prof. Jarugu Narasimha Moorthy**

Director,

Indian Institute of Science Education and Research, Thiruvananthapuram



The Storage MAP is a pool of 16 investigators from 15 pioneer research institutes to leverage the expertise and knowledge towards solid-state battery research. I am delighted to share that the consortium capacitates excellence and innovation in advanced materials research. We, at IISER TVM, deem it a pleasure to house the centre at our lush green campus and are looking forward to breakthrough research findings in this emerging field.

Dr. M. M. Shaijumon Center Head & Administrative PI Indian Institute of Science Education and Research, Thiruvananthapuram

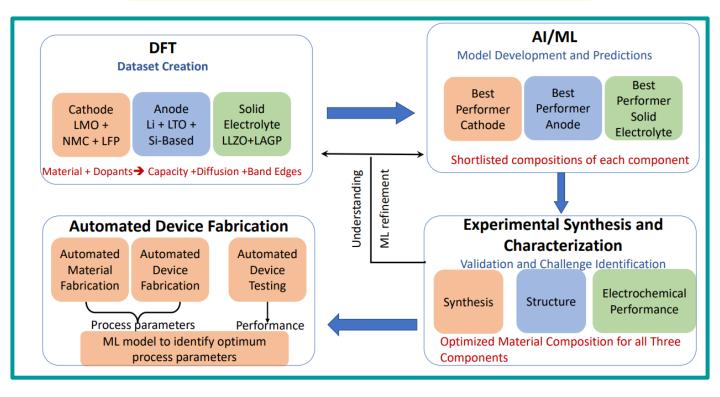


ICMAP-storage consortium will enable the rapid paced transformation and subsequent commercialization of solid-state technologies. This whole development of technologies is planned to get accelerated by machine learning and artificial intelligence. Under this consortium, a team of 16 researchers from all part of country have joined hand together to make India a self-reliant country in advanced energy storage technologies. I am sure under the aegis of Mission innovation, DST-ICMAP consortium would lead to a transformative change in adoption of clean energy solutions. Dr. Yogesh Kumar Sharma

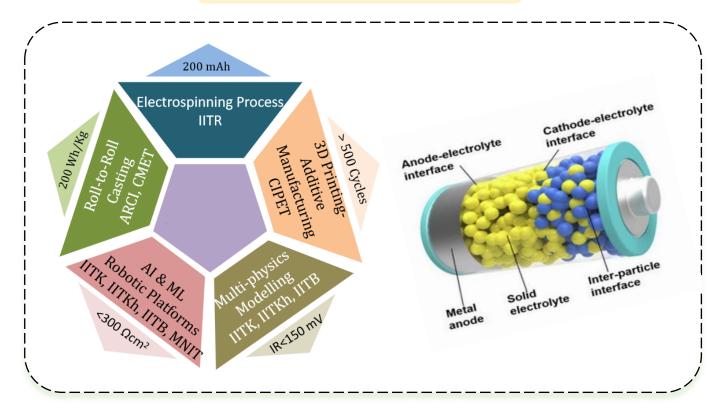
Dr. Yogesh Kumar Sharma Center Lead PI Indian Institute of Technology Roorkee

Research Highlights

AI/ML Assisted Accelerated Material Design



Device specifications



Facilities at the partnering institutes







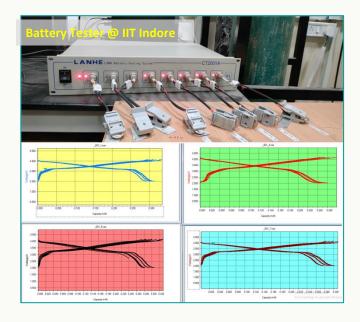


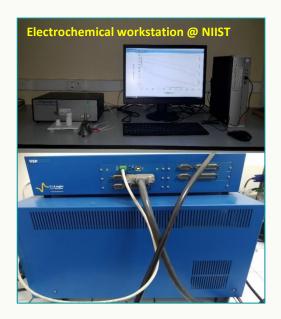




Facilities at the partnering institutes













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