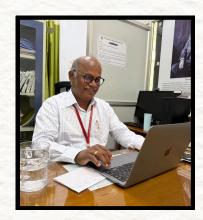


#### **PRINCIPAL**



**HEAD OF THE DEPARTMENT** 



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#### **ACKNOWLEDGEMENT**

Reading is not merely an act, it is a journey across time, cultures and discipline, it is through this journey that knowledge becomes wisdom, and wisdom has the power to reshape the society. Every technological advancement in the field of energy, electronics, communication and medicine finds its roots on the fundamental insights of physics. From the tiniest quantum particles to the vastness of cosmic phenomena, physics continues to illuminate the path of innovation. We the department of physics is eager and excited to present our newsletter **Q-AATRAL** which signifies the Quantum of Energy that drives the realm of science and technology.

Through this newsletter, we aim to highlight the key developments within our department, from cutting-edge research in frontier areas of science to the sate-of-the-art facilities housed in various laboratories of our department. It features insightful articles contributed by research scholars, with every page reflecting the curiosity, creativity, and commitment that define our academic community.

Our sincere thanks to the Management and Principal Prof. Dr. L. Ashok Kumar for their unwavering support and encouragement. We extend our sincere gratitude to the Head of the Department of Physics Prof. Dr. M. Mahendran for his strategic foresight and commitment. His dedication and commitment played a pivotal role in paving the way for the continued development and sustainable growth of the department.

A sincere thanks to the editorial team, faculties and research scholars of the department for their invaluable support and contributions. Their dedication and involvement played a vital role in the successful outcome of Q-AATRAL, reflecting the collaborative spirit and academic excellence that define the department of Physics. Together we continue our journey in the field of science thereby striving to expand frontiers of knowledge and contributing towards technological development for the upliftment of our Society.

Thank you for all the valuable Contributions.

**NEWSLETTER TEAM** 

#### **OUR COLLEGE**

Thiagarajar College of Engineering (TCE) is as a Government Aided Autonomous Institution, established in 1957 by the philanthropist Late Karumuttu Thiagarajan Chettiar. TCE is affiliated to Anna University, Chennai, and approved by All India Council for Technical Education (AICTE). TCE offers a wide array of Undergraduate, Postgraduate and Ph.D. Programs across various disciplines of Engineering, Architecture and Science. Each academic Department at TCE is dedicated to a specific theme, fostering synergy between faculty and students in academic and research endeavours. The college maintains active industry collaborations with leading global organizations. TCE's active participation in the Technical Education Quality Improvement Programme (TEQIP) under the National Project Implementation Unit (NPIU) of the Ministry of Human Resource Development (MHRD) has led to innovative teaching and learning processes, faculty development programs, industry-supported research activities, and good governance initiatives. The institution's programs have been accredited by NBA since 1998, indicating compliance with quality standards in technical education. The programmes offered at institution has garnered numerous accolades, including accreditation by NAAC with a CGPA of 3.56 (out of 4.0) with A++ Grade in Cycle 2. The major objective of the institution is to plan and implement programme of education in Engineering and allied Sciences, to promote research and disseminate knowledge for the upliftment of our society.

#### **VISION AND MISSION (STRATEGIC PRIORITIES OF TCE)**

- Achieve academic excellence in Science, Engineering and Technology through dedication to duty, commitment to research, innovation in learning and faith in human values.
- Enable the students to develop into outstanding professionals with high ethical standards capable of creating, developing and managing global engineering enterprises.
- Fulfil expectations of the society and industry by equipping students with state of art technology resources for developing sustainable solutions.
- Achieve these through team efforts making Thiagarajar College of Engineering, the socially diligent trend setter in technical education.

#### ARCHITECT OF TCE

Kalaithanthai Karumuttu Thiagarajan Chettiar, is a great visionary with a mission. He was bestowed with the moral and social responsibility of building up this institution with an objective of serving the society. A staunch nationalist and a great industrialist, he led a life of sacrifice. He was as an exceptional educationalist, who had a keen eye on transforming lives through education. As an exceptional social savant, he left his footprints in the sands of time in all facets of his social life. Being a discrete reader, his passion for language was evident as he possessed a great command over the language of Tamil. As a generous philanthropist through his righteous deeds, he continues to live in the hearts of many. Kalaithanthai Karumuttu Thiagarajan Chettiar is a holistic personality with spiritual aura and soul.

#### DEPARTMENT OF PHYSICS

Physics department was established in the year of 1957. Department of Physics in collaboration with other engineering department of TCE offers Ph.D program in various specialization such as Smart Materials, Thin Film Materials and Nano Materials. The Department is supported by FIST program of DST, New Delhi. The department also collaborates with industries, academic and professional bodies and was actively engaged in many technology development programs and sponsored project from BRNS, DRDO, DST, ISRO, CSIR and AICTE.

#### **VISION**

World class quality technical education with strong ethical values.

#### **MISSION**

- The technological revolution owes its drastic development to advances that depend strongly on progress in materials science. Keeping this in mind the department of Physics sets the mission.
- To establish infrastructure to develop novel materials essential for competitive research.
- To provide opportunities for new eyes to observe and new hands to manipulate at micro and nano scales that enable new insights into systems of recognized importance and the exploration of completely new regimes.
- To foster strong link with the multifaceted laboratories, diverse interdisciplinary laboratories of Science and Engineering disciplines.

#### MESSAGE

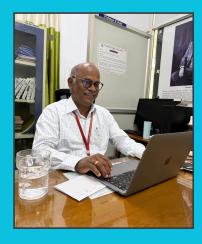
#### **PRINCIPAL**



It is a great pleasure for Thiagarajar College of Engineering to unveil **Q-AATRAL**, the newsletter of the Department of Physics. This publication reflects the department's dynamic initiatives by showcasing its research milestones, creative endeavors, spirited energy, and innovative achievements.

**Q-AATRAL** is not merely a chronicle of events—it serves as a testament to the department's ongoing scientific excellence and impactful accomplishments. I extend my sincere appreciation to all contributors for their dedication and commitment in bringing this publication to life.

#### HEAD OF THE DEPARTMENT



I am eager to provide comprehensive scientific support to our department for the publishing of our newsletter, **Q-AATRAL**, which signifies Quantum of Energy and integrates the realms of science and technology. We are well-acquainted with emerging frontier technologies, such as Quantum Computing, where materials at the submicroscopic size are essential for the sustainable development of society.

**Q-AATRAL** examines the activities conducted in our department, primarily emphasizing research and development. The young individuals in our department are excelling in both academics and research. I wish for the successful and consistent publication of this **Q-AATRAL** newsletter featuring groundbreaking content.

#### STAFF EDITOR



I express my sincere gratitude and acknowledge the dedication of the editorial team, faculty members, and research scholars of the Department of Physics. This newsletter, **Q-AATRAL**, serves as a showcase of the department's research activities, advanced facilities, and a variety of academic and outreach initiatives. Physics has always been a source of inspiration and a strong foundation for the development of technological advancements. May this newsletter continue to inspire and reflect the spirit of innovation that drives our department forward.

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VI



#### **Dye Pollution and Its Environmental Impact**

In ancient times people used organic dyes, so the environment was not more polluted, but in the last 200 years people have used inorganic dyes this is more dangerous for humans and nature. synthetic dyes are used in industries such as textiles, paper, leather, plastics, cosmetics, and food processing most commonly in the textiles industry. In our India have more textile industries, the rivers was more pollutant. The textiles industry consumes dyes to a greater extent than all other industries combined. In textile dyeing operations, wastewater produced may carry away 10% to 15% of the dye. Given that synthetic dyes are typically toxic, carcinogenic, and resistant degradation, dye effluents contribute to environmental pollution and to the amounts of synthetic chemicals in the environment. Water in aquatic environments with dye loses light penetration; which limits photosynthesis and dissolved oxygen in the water. These chemical will disrupt and alter the aquatic life in the surrounding environment and ecosystems resulting in fewer healthy ecosystems, and biodiversity. Aquatic ecosystems are challenged when wastewater from a variety of industries contain high dye loads because a large number of dye molecules and their metabolite molecules can exist for varying lengths of time in wastewater without being degraded.

Contaminants that are not treated by standard biological treatments can remain in water for an extended time. Because of this, dye degradation techniques should be prioritized. The decomposition or removal of colour molecules from polluted water through physical, chemical or biological processes is called dye degradation. Dye degradation methodologies are important natural technologies for



P. Sundararajaperumal Research Scholar

wastewater treatment and environmental sustainability. Therefore, use of clean water to protect water systems in a sustainable management agenda do have some reliance on practices of dye degradation. These regulations determine the health of ecosystems and communities that rely on these water systems, alongside regional water initiatives.

#### Mechanisms of Dye Degradation

Dye degradation can occur via a variety of mechanisms, each one with their own strengths. One of the most researched, as well as most effective, mechanisms is photocatalytic degradation. This mechanism of dye degradation takes advantage of a semiconductor material (often TiO<sub>2</sub> or ZnO). When this semiconductor is exposed to UV or visible light, the photonic energy activates the semiconductor surface, which in turn creates electrons (e-) in the conduction band and holes (h+) in the valence band upon irradiation. These charge carriers can then be used for redox reactions

- Holes (h\*) react with water molecules to produce hydroxyl radicals (•OH).
- Electrons (e<sup>-</sup>) reduce molecular oxygen to produce superoxide radicals ( $\bullet$ O<sub>2</sub><sup>-</sup>).

These reactive oxygen species (ROS) can react with dye molecules, disrupt their chromophores, and eventually degrade them into smaller and safer forms. The complete reaction can be written as:

$$M + hv \rightarrow e^{-} + h^{+}$$

$$h^{+} + H_{2}O \rightarrow \bullet OH + H^{+}$$

$$e^{-} + O_{2} \rightarrow \bullet O_{2}^{-}$$

### OH / ${}^{\bullet}O_{2}^{-}$ + dye $\rightarrow$ degradation products (CO<sub>2</sub>, H<sub>2</sub>O<sub>2</sub>, inorganic salts)

Lastly, the family of Advanced Oxidation Processes (AOPs) is another very effective option to consider, as they leverage the powerful and nonselective oxidizing ability of hydroxyl radicals. Some of the more mainstream AOPs with practical utility for dye decolorization include

Some examples include:

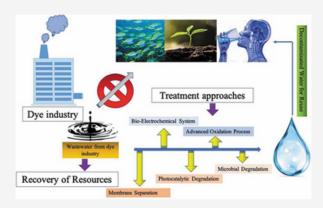
- Fenton and photo-Fenton processes: Involves iron salts (Fe2+ or Fe3+) and hydrogen peroxide (H2O2), often under UV sources to produce
   OH radicals.
- Ozonation: Ozone (O3) decomposes in water forming hydroxyl radicals and also reacts directly with dye molecules.
- Electrochemical oxidation: Employs electrodes to generate ROS on electrode surfaces to degrade dyes via electrochemical redox reactions sought from aqueous waste.

Not only do these techniques provide excellent degradation efficiency, but many can be manipulated in real-time for wastewater treatment, which makes them appealing for the industrial treatment process. The success of the AOPs can depend on operational parameters by manipulating pH, light intensity, catalyst concentration, and dye type.

#### **Applications, Challenges, and Future Perspectives**

The successful implementation of dye degradation methods has enormous benefits for managing industrial wastewater, primarily for the textile, paper, and printing sector. Industries can effectively manage effluent color and toxicity with at least some degree of compliance with relevant environmental regulations, recycling into other industrial processes, and safeguarding public health. Newest iterations are working toward producing innovations that combine dye degradation into a sustainable energy source, such as producing green hydrogen.

As an example, integrating photocatalysis with water splitting can remove pollutants while simultaneously generating hydrogen, yielding double-duty benefits.. Additionally, new smart hybrid systems are being developed to effectively incorporate multiple treatment methods enhance their efficiency, operational costs, and manage a far broader range of pollutants: approaches photocatalytic with membrane filtration; or, biological treatment. These smart hybrid systems show promise for existing and future large-scale systems for real world application.



Source: Shindhal et. al., Bioengineered, 12(1), 70–87 (05.08.2025, 02.12 pm)

#### Future research is directed towards

- Creating photocatalysts that can be activated using visible-light sources, so we can take advantage of natural sunlight, rather than having to use artificial UV sources.
- Developing environmentally sound materials including photocatalysts made from biowaste and composites made from natural minerals.
- Implementing renewable energy into the dye degradation systems to reduce fossil fuels.
- Moving from laboratory to pilot plant and commercial treatment facilities.

While biological degradation is environmentally sound, it will need to be optimized, along with genetic modification to enhance the degrading efficiency of complex dyes. A multidisciplinary team will be needed to develop systems to treat these dyes. With innovation and collaboration, it certainly let industry sustain itself long term and solve the global agenda of environmental and sustainability issues over dwindling resources.

# Supercapacitors and Supercapatteries: The Future of Energy Storage

#### Introduction

It began with a moment, one that many of us have likely experienced in our increasingly electrified world. The power flickered. The lights dimmed. A phone left charging overnight sat untouched by the current that should have surged through its cord. In that moment of silence and stillness, an engineer, sitting by the window and watching the blades of a distant wind turbine slow to a stop, asked the question: What if we could store energy better? Not just more of it, but faster, cleaner, and with fewer compromises? This is not just one person's question. It is a global one. As the world faces a dual crisis of surging energy demand and the urgent need to decarbonize, we find ourselves at a critical crossroads. Renewable energy sources like solar and wind have promised cleaner, greener alternatives to coal and gas. But while they bring hope, they also introduce a new set of challenges. Chief among them? Intermittency. The sun doesn't always shine, and the wind doesn't always blow. And yet our need for power steady, reliable, and fast never stops.

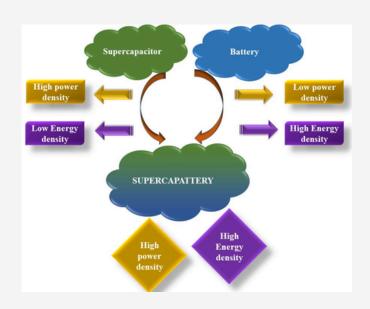






A. Anusuya & K. Aruna Devi Research Scholars

To bridge this gap between nature's rhythm and our relentless demand, scientists and engineers around the world are racing to innovate better energy storage systems. the go-to solution, their limitations are increasingly hard to ignore: slow charging speeds, limited lifespans, and environmental costs from mining and disposal.



Enter a new generation of storage heroes: supercapacitors and the cutting-edge supercapatteries. These technologies represent more than just upgrades they symbolize a fundamental shift in how we think about energy storage. Supercapacitors, known for their lightning-fast charge and discharge capabilities, are already finding roles in everything from regenerative braking systems to space tech. Meanwhile, supercapatteries hybrid devices that aim to merge the best qualities of supercapacitors and batteries are pushing the boundaries of what's possible. This article explores the promise and potential of these groundbreaking technologies. From the laboratories where they are being engineered to the grid systems and electric vehicles they may one day power, we delve into the science, the vision, and the people who are working to redefine our energy future. Because when innovation is sparked by necessity and inspired by a flicker in the dark the result can be nothing short of revolutionary.

#### **Supercapacitors**

Supercapacitors sometimes called ultracapacitors are a fascinating breed of energy storage devices that challenge everything we think we know about how energy can be stored and released. conventional batteries, which depend on slow, often messy chemical reactions to produce electricity, supercapacitors operate on a much more elegant and rapid principle: electrostatic charge storage. Imagine energy not being coaxed from sluggish internal chemistry, but instead, leaping to attention in an instant, ready to flow. That's the magic of supercapacitors. At their core, these devices are deceptively simple: two electrodes, an electrolyte, and a separator. Charges rapidly accumulate on the surface of each electrode, forming what scientists call an electric double layer a tightly packed arrangement of positive and negative charges poised and ready to move. Because this process is purely physical and doesn't involve breaking or forming chemical bonds, it is not only extremely fast, but also highly reversible. That means supercapacitors can be charged and discharged hundreds of thousands even millions of times with barely any loss in performance.

But like any technology, supercapacitors have their Achilles' heel: energy density. They simply don't hold as much energy as traditional batteries. Think of it this way if a lithium-ion battery is a water tank that slowly releases its stored contents over hours, a supercapacitor is more like a firehose: intense, powerful, but shortlived. Because of this, they've historically been relegated to niche roles places where bursts of energy are more important than long durations. You'll find them hidden in regenerative braking systems, where they quickly store and release energy as a vehicle slows down, or in backup power supplies that need to kick in instantly during power interruptions. Despite these limitations, the appeal of supercapacitors continues to grow. Their ability to deliver power at lightning speed, combined with lifespans that outlast any battery, make them increasingly attractive option for a future where energy needs to be not just stored, but ready at a moment's notice. As researchers work to increase their energy density through new materials, hybrid systems, and smarter designs supercapacitors may soon find themselves moving from the sidelines into center stage.

#### **Supercapattery**



Source: Sciencedirect.com (07.08.2025,11:00am)

To tackle the long-standing challenge of energy density in supercapacitors, researchers around the world have turned to a creative solution: hybrid energy storage devices that blend the strengths of both batteries supercapacitors. At the heart of this innovation lies a new class of devices known supercapatteries a name that reflects exactly what they are: part supercapacitor, part battery. These aren't just a compromise they're an evolution. Supercapatteries are designed to strike the perfect balance between two essential but often opposing qualities in energy storage: power and capacity. On a technical level, they work by combining materials that support both capacitive (fast, surface-level energy storage) and faradaic (slower, chemicalbased energy storage) processes. This dual mechanism means they can deliver rapid bursts of power when needed just like a supercapacitor while also storing enough energy to keep things running longer, much like a traditional battery.

It's a bit like having the best of both worlds in a single device: the speed and durability of a sprinter with the endurance of a marathon runner. And the potential applications are as exciting as the technology itself.

Supercapatteries are especially promising in fields where energy demands are complex and constantly shifting. Take electric vehicles, for example they need quick bursts of energy for acceleration, but also a steady supply for longer drives. Or grid stabilization systems, which must respond instantly to fluctuations in power supply and demand. Even portable electronics stand to benefit, as supercapatteries could offer faster charging and longer usage times in a single, compact package.

As the technology matures, supercapatteries may very well become the go-to solution in a future that demands more from our energy systems than ever before faster, cleaner, and smarter.



Source: Sciencedirect, (05.08.2025, 11.00 am)

#### **How Do They Work?**

Central to the performance of both supercapacitors and supercapatteries is the choice of materials used for the electrodes and electrolytes. Nanostructured materials have opened up vast possibilities for improving energy storage. Carbonbased materials such as graphene and carbon nanotubes are extensively used due to their high surface area and excellent conductivity, which enhance the capacitive behavior of electrodes. Meanwhile, transition metal oxides like manganese dioxide (MnO) and nickel hydroxide (Ni(OH)) are often included to add battery-like properties. Conducting polymers have also shown promise, offering flexibility and tunability in electrochemical behavior.

The choice of electrolyte is equally critical, as it influences the device's voltage window, operating temperature, and overall stability. Advanced electrolytes, including ionic liquids and organoaqueous systems, are enabling supercapacitors and supercapatteries to operate safely at higher voltages and in wider environmental conditions. These innovations are not only pushing performance limits but also helping to make these technologies more commercially viable.



#### **Birth of Computational Material Science:**

While reading about the quantum theory, I found myself wondering how something so tiny and invisible could follow such strange yet beautiful rules. This curiosity led me to explore the language that describes the atomic world- the wavefunction. In quantum mechanics, the wavefunction describes the entire state of a system. This means, for example, when an atom has an electron revolving around the nucleus, the state wavefunction is used to describe the electron's behavior in terms of its total energy. You can imagine holding an atom in your hand with electrons around it. If we have N number of electrons, and each electrons has 3 Spatial coordinates, the total wavefunction depends on 3N variables. That's an enormous amount of data for even a small system! We can predict an electron's behaviour using the time-dependent Schrödinger equation:

 $H\psi(r)=E\psi(r)$ 



Source: Humankind and Science (05.08.2025, 10.14 am)

This equation works well for one-electron systems like the hydrogen atom.



S. Reema Sagitha Research Scholar

However, when dealing with a many-electron system, the equation becomes:

$$H\Psi(r_1, r_2, ..., r_N) = E\Psi(r_1, r_2, ..., r_N)$$

In such cases, solving this becomes computationally intensive and often impractical. Predicting the behaviour of electrons accurately can take an immense amount of time, even days or years for large systems.

#### From Wavefunction to Electron Density:

To tackle this challenge, scientists in the 1920s, notably Enrico Fermi and others, introduced a new approach: using electron density instead of the wavefunction. For a day-to-day life example, imagine a pomegranate, its difficult to count the small seeds inside the fruit-like the complex wavefunction that tracks each electron. But its much easier to count the number of fruits in a box-just like electron density simplifies the whole system.

#### **Untangling the Many-Body Puzzle:**

The complexity of the many-body problem arises from how electrons interact with each other through mutual repulsion. While solving the Schrödinger equation is straightforward for a single electron, multiple electrons form a complex network of interactions. This simplification allows for easier calculation of electronic structure. It's like analyzing a movie scene by freezing the background (nuclei) to focus only on the fast-moving car (electrons).

Following this, the Hartree-Fock (HF) method was developed a major advancement. It assumes that each electron moves independently in an average field created by all other electrons, rather than computing interactions between every pair. Imagine a crowd in a public square: instead of tracking individual interactions, HF assumes everyone moves based on the average flow of the group. Though this model is a simplification, it works remarkably well for many systems.

#### **Pillars of Density Functional Theory:**

Modern DFT took shape in the 1960s through the work of Walter Kohn, Pierre Hohenberg, and Lu Jeu Sham. The foundation of DFT rests on two critical theorems proposed by Hohenberg and Kohn:

- (1) Uniqueness Theorem: Given the ground-state electron density, all properties of the system including the external potential and total energy are uniquely determined.
- (2) Variational Principle: The ground-state energy of a system is the minimum value of an energy functional, achieved when using the correct ground-state electron density.

The variational principle is particularly important and is rooted in classical physics similar to Jacobi's principle, where nature always follows the path of least action. These theorems marked a significant shift in quantum mechanics, making DFT a powerful tool in computational science.

However, while these theorems provided a theoretical framework, they didn't offer a practical method to compute electron density. This gap was filled by Kohn and Sham, who introduced the Kohn-Sham equations.

#### The Kohn-Sham: Heart of DFT

Kohn and Sham suggested that instead of solving the full interacting many-electron problem, we can simulate a system of non-interacting electrons moving in an effective potential. This potential is constructed such that it produces the same electron density as the real system.

The Kohn-Sham equation is given by:

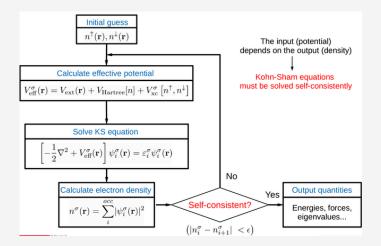
$$[-\nabla^2 + V_{eff(r)}] \psi_i(r) = \varepsilon_i \psi_i(r)$$

Where the effective potential is

$$V_{eff} = V_{eN} + V_H + V_{xc}$$

where,

- V<sub>ext</sub>: external potential
- $\bullet$  V<sub>H</sub>: Hartree (classical electron-electron) potential
- V<sub>xc</sub>: exchange-correlation potential
- V<sub>eff</sub>: effective potential



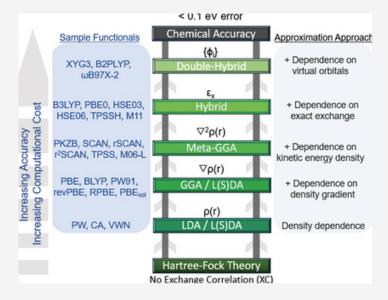
Flow Chart of the Self-Consistent Field (SCF) Cycle

Source: SIESTA Project Documentation, 2024 (05.08.2025, 11.20 am)

Since  $V_{\text{eff}}$  depends on the electron density, which depends on the orbitals from the equation, the answer necessitates an iterative process known as the Self-Consistent Field (SCF) method:

- (a) Estimate the electron density first.
- (b) Determine V<sub>eff</sub> based on the guess.
- (c) Solve Kohn-Sham equations to get new orbitals.
- (d) Refresh the density of electrons.
- (e) Repeat the process until the input and output densities are equal, or self-consistent.

The exchange-correlation term  $(V_{xc})$  is the most challenging part to approximate accurately. Finding a suitable form for the exchange-correlation functional  $(V_{xc})$  is one of the difficulties in DFT.



#### Jacob's Ladder of Density Functional Theory

Source: A. Badreldin et al., ResearchGate, 2023 (05.08.2025, 12:44 pm)

As a result, John Perdew developed the idea of Jacob's Ladder, which depicts the hierarchy of progressively more complicated approximations: Local Density Approximation (LDA), Generalized Gradient Approximation (GGA), Meta-GGA. The accuracy of DFT results heavily depends on the choice of exchange-correlation functional.

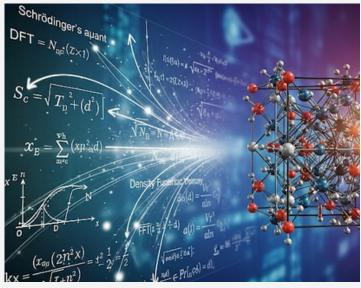
Note: Walter Kohn received the Nobel Prize in Chemistry in 1998 for his contributions to the development of Density Functional Theory, a development which revolutionized the study of electronic structures.

#### A New Era of Materials Discovery:

Computational materials science has revolutionized how we discover and design new materials. Today, alongside laboratory experiments, we use computer simulations to understand how materials behave at the atomic level. This advancement allows researchers to develop improved solar cells, batteries, sensors, and even medical materials more efficiently. Before building them in reality, scientists now model these materials on computers using widely used software packages like:

- VASP
- Quantum Espresso
- WIEN2k

These tools make material discovery faster, more cost-effective, and precise, helping researchers bring next-generation technologies to life.



### Hydrogen Unleashed: Unlocking Clean Energy from Every Drop of Water

#### Introduction

In recent decades, the rapid growth of the population has led to a sharp increase in energy demand and use, which is primarily a net contributor to environmental pollution. Simultaneously, the conventional sources of energy have been decreasing, raising concerns over energy security. Researchers have been working hard to reduce energy and environmental problems by identifying alternatives to using oil, gas, and coal. Among these choices, hydrogen (H<sub>2</sub>) is increasingly being touted as a clean and efficient fuel source due to its high energy content and sustainability aspects. For hydrogen to join a hydrogen economy, it is essential to find inexpensive and efficient ways to produce, store, and transport it. Researchers are working in many different global research hubs to examine ways to efficiently, cheaply, and in large volume do water splitting, either in photocatalysis, electrocatalysis, or photoelectrochemical systems.

#### Photocatalytic water splitting

Photocatalysis harnesses sunlight to activate semiconductor materials that can split water. The most recognized photocatalysts include  ${\rm TiO_2}$ , g-C<sub>3</sub>N<sub>4</sub>, WO<sub>3</sub>, and various perovskite materials, which function similarly. These photocatalysts utilize sunlight to produce electron–hole pairs, enabling water-splitting reactions. Recently, there have been several advances in photocatalysis, including:

- Z-scheme photocatalytic systems enhance redox potential by mimicking natural photosynthesis.
- Doping with rare earth elements like cerium (Ce) and lanthanum (La) improves visible light absorption



S. Pon Lakshmanan, Research Scholar

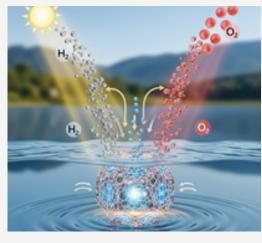




K. Kaviya & K. Nithya Research Scholars

• Heterojunction engineering helps better separate charge and reduce recombination.

Nanostructures, including nanorods and nanosheets, increase surface area and active sites.



Source: Vitaponix.com (05.08.2025, 12.35 pm)

These advances are very significant and show progress toward photocatalysis for practical production of hydrogen on a large scale

#### **Electrocatalytic Water Splitting**

In electrocatalysis, electricity is used to split water into hydrogen and oxygen in an electrolyzer. This process involves two main reactions:

- Oxygen Evolution Reaction (OER)
- Hydrogen Evolution Reaction (HER)

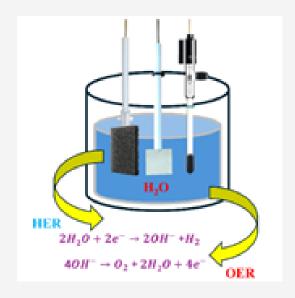
While noble metals like Pt (HER) and IrO<sub>2</sub> (OER) are effective catalysts for electrocatalytic water splitting, they are expensive and rare. Therefore, researchers are focusing on alternative catalysts such as nickel-iron oxides (NiFe<sub>2</sub>O<sub>4</sub>), Cobalt-based catalysts (Co<sub>3</sub>O<sub>4</sub>, Co-P), and sulphide and phosphide materials (MoS<sub>2</sub>, Ni<sub>2</sub>P). These suggest the potential for low-cost, scalable hydrogen production heterojunction engineering to achieve charge separation and suppress better recombination. NNano-structuring such as using nanorods and nanosheets to maximize surface area active sites. enhances provide more photocatalytic performance.

#### Photoelectrochemical (PEC) Water Splitting

PEC water splitting incorporates efficiencies of both photocatalysis and electrocatalysis to produce an integrated system. In a PEC cell, a photoactive electrode utilizes sunlight to facilitate the watersplitting reaction directly on its surface.

Recent progress towards PEC water splitting includes:

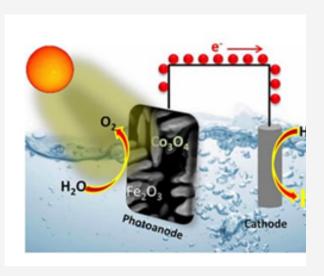
- The development of advanced photoanode materials with BiVO<sub>4</sub> and Fe<sub>2</sub>O<sub>3</sub>.
- The utilization of tandem cell setups with different semiconductors to increase light absorption.
- Also, co-catalyst layers to simultaneously improve both stability and the efficacy of the photocatalytic process.



#### **Catalyst Engineering and Synthesis Methods**

Researchers have developed many synthesis methods to improve catalyst performance toward water splitting. Some of the synthesis methods include: Hydrothermal and solvothermal synthesis

- ü Sol-gel processes
- ü Electrospinning
- ü Atomic Layer Deposition (ALD)



All of these methods can be used to finely tune the morphology, particle size, and surface properties of the catalyst to improve activity and stability. Also, many approaches like doping, defect engineering, and composites are widely used to enhance light absorption, catalytic activity, and charge transport.

Doping, defect engineering, and composites are widely used to improve light absorption, catalytic activity, and charge transport.

#### **Advanced Characterization Techniques**

To understand properties of catalysts and to study how they perform, researchers use advanced characterization techniques, such as:

- X-ray Diffraction (XRD) measures crystal structure
- Scanning and Transmission Electron Microscopy (SEM/TEM) – examines the morphology and nanostructure
- X-ray Photoelectron Spectroscopy (XPS) reveals chemical composition and oxidation states on the surface
- UV-Vis Spectroscopy determines the optical and absorption properties
- Electrochemistry techniques such as Linear Sweep Voltammetry (LSV), Electrochemical Impedance Spectroscopy (EIS), and Turnover Frequency (TOF) – yield insights into catalytic activity and stability

These characterization methods, therefore, provide useful information about catalysts' structure–activity relationships and can help researchers develop more efficient materials.

#### Role of AI and Computational Modelling

Artificial intelligence (AI), including machine learning (ML), as well as computational techniques such as Density Functional Theory (DFT), are transforming the space of suitable materials for water-splitting. Specifically, the tools help with the:

- Prediction of electronic band structures to determine the suitability of the material.
- Screening of materials in large libraries to find candidate materials.
- Optimization of reaction parameters for higher performance.
- Determination of stable catalyst structures for catalyst operation conditions.

Overall, a data-driven approach is speeding up the experimental cycle, enhancing prediction quality, and accelerating the development of next-generation catalyst solutions.

#### **Worldwide Hydrogen Developments**

Countries around the world are investing in hydrogen energy source development to enhance sustainability and lower carbon emissions. Some notable initiatives are:

- India initiated the National Green Hydrogen Mission (2023).
- Germany approved a detailed National Hydrogen Strategy.
- Japan and South Korea-Creating substantial hydrogen infrastructure and capabilities.
- Australia-Planning the production and exporting of green hydrogen.

These initiatives are necessary steps along the road to a lower-carbon, hydrogen-based global economy.

### Challenges and Future Outlook Despite progress, water splitting still faces challenges:

- High cost of efficient catalysts
- Poor long-term stability
- Complex device integration
- Scalability of lab-scale methods
- Future directions include:
- Developing earth-abundant, low-cost catalysts
- Creating self-healing materials
- Designing 3D-printed electrolyzer systems
- Using AI for predictive material design

  Continued interdisciplinary research will play
  a vital role in bringing water-splitting
  technologies closer to commercialization.

#### Conclusion

Water splitting is an exciting and environmentally friendly way to produce green hydrogen. Advances in materials science, nanotechnology, and electrochemical engineering continue to push the boundaries quickly. Greater collaboration between academia and industry will help solidify a hydrogen future that is rapidly evolving from vision to reality-potentially transforming the global energy landscape.



#### Introduction

In the era of computer technologies, the source of development is hiring years by years, is where quantum computing accomplishes. Regular computers that operate with bits (0 or 1) operate differently than quantum computers that operate with qubits—able to be 0 and 1 simultaneously. That special ability, superposition, creates a new dimension of problem-solving. The fact that entanglement, a quantum phenomenon, binds qubits such that their states affect one another even at great distances, adds to its excitement.

These features, when combined with quantum interference, allow quantum computers to identify patterns and solutions far more quickly than even the most powerful supercomputers available today. This translates into improved diagnostics, quicker medication development, and cleverer treatment strategies in medicine.





C. Thirisha Research Scholar

How Quantum Power Transforms Patient Care Did you know that each human body generates more than 1 terabyte of health information annually? From genomic sequences and highresolution MRI images to real-time tracking from wearable devices, medicine is immersed in an ocean of intricate, high-dimensional data. Though traditional computers strain to catch up, their limitations reveal themselves when it comes to modeling the interactions between thousands of molecules, forecasting disease progression, or tailoring treatment plans to individuals. Qubits in quantum computers exist in numerous states at the same time, allowing them to handle massive quantities of data with incredible efficiency. Consider the possibility of testing how a medication molecule interacts with a cancer cell in minutes rather than weeks. Scientists can utilize this capacity to uncover the underlying causes of sickness, find patterns that would otherwise go undetected, and even predict how a patient will react to a medicine before it has been clinically trail or administered.

In conclusion, quantum computing isn't just a science-fiction device; it's quickly becoming the next frontier in customized medicine, enabling better, quicker, and more secure healthcare.

### VQE simulates molecules and accelerates drug development.

Quantum computers can model molecules at an atomic level with algorithms such as the Variational Quantum Eigensolver (VQE). This helps scientists predict how a drug will behave inside the body—before physical lab testing begins. Such simulations reduce the trial-and-error process, accelerating the time it takes to move from discovery to clinical use. In the future, we may even see quantum-designed molecules that are custom-built for specific types of cancer or genetic disorders.

### Talk about quantum-enhanced MRI, CT, and cancer image recognition.

Quantum machine learning can improve the accuracy of medical images like MRI and CT scans. It can remove background noise, sharpen blurred regions, and **even detect microscopic tumors** that are otherwise hard to see. This helps radiologists and AI systems make faster, life-saving decisions. By converting pixel values into quantum states—a method called amplitude encoding—quantum systems process imaging data faster than traditional systems, reducing diagnostic delays.

#### Focus on genome data, DNA, custom treatments.

Every person's DNA is different. With quantum computing, large-scale **genomic analysis** becomes faster and more detailed, enabling doctors to create **custom treatments** based on a patient's unique genetic profile. This means fewer side effects, more targeted therapies, and better results. In future, quantum AI may even predict diseases before symptoms appear, based on subtle DNA or protein changes.

#### QAOA and optimization in healthcare

QAOA can be useful for optimizing physician scheduling in health care, by helping strike a balance between workload, accommodating preferences or expressing constraints, as well as avoiding potential clashes.

Resource allocation (beds, equipment, staff) is important in health care operations. QAOA has potential applications in drug discovery. We can use QAOA to model the molecular interactions of drugs and predict their behavior, which could speed up the drug discovery process.

In the field of radiation therapy, we can apply QAOA to help design treatment plans, helping to maximize delivery of treatment to cancerous cells while minimizing damage to healthy tissue.

#### **Quantum Breakthroughs to Watch!**

Through the National Quantum Mission (NQM), India is investing ₹6,000 crores (approx. \$730 million) to develop quantum technologies for fields like biotechnology, cancer

#### **Software Empowerment**

Simulation tools like Qiskit (IBM) and Cirq (Google) are being actively utilized to create quantum circuits with the goal of enhancing illness diagnostics and examining molecular interactions in the quickly developing field of quantum healthcare. The ground state energy of chemicals linked to cancer may be studied because to algorithms like the Variational Quantum Eigensolver (VQE).

Advanced simulation programs like Gaussian, VASP, and Quantum ESPRESSO are frequently used in material research to calculate electrical characteristics and simulate crystal structures. Python-based platforms like ASE (Atomic Simulation Environment) facilitate this by enabling simplified automation and management of simulation processes.

Matplotlib, Plotly, and ParaView are visualization tools used to analyze and display complicated quantum and materials data. Meanwhile, optimization and hybrid quantum-classical algorithms benefit from libraries like SciPy and PennyLane, driving advancements in quantum machine learning.

### The Road Ahead: Quantum Healthcare Is Just Beginning

Technology and computing are transforming the way we provide healthcare. Consider how society would change if it were possible to identify a disease before symptoms appear or if a third-generation medication could be created in a few months as opposed to years. Yes, they can. Because of their capacity to handle large, complicated information, quantum computers are opening up previously unimaginable possibilities.

Quantum computers, for example, can assist in the deciphering of genetic abnormalities in cancer. In order to provide user-specific therapies, they can also model molecular interactions.

With finer tools, greater simulations, and insights that might save lives in amazing new ways, quantum systems can analyze in ways that traditional computers cannot. As many tech businesses and research labs across the world scramble to invent the future, quantum-powered computation and technology are transforming the way we provide healthcare. In healthcare, "someday" is giving way to "shortly." We are approaching a time when science fiction becomes medical reality thanks to cooperation between physics, medicine, and artificial intelligence.

"Quantum computing is giving healthcare a new language—one written in probability, precision, and hope."



### Shaping the Future with Shock-Responsive Materials

#### Introduction

Have you ever thrown a rock into a pond and watched as the ripples travelled away from the site of the rock? Those ripples are a wave traveling through water. If you then try to imagine something like a wave propagating through solid or gas but travel faster and stronger to form a special type of wave called a shock wave, you would then beginning to see the direction we are headed.

Shock waves might feel abstract or related to scifi, but they do exist and operate in various contexts - including medical treatments, industrial processes, and approaching our understanding of explosions. What is even more interesting is classes of materials that can change their own structure when they experience impacts associated with shock waves. We call those materials phase-transforming materials, and they offered exciting opportunities for the future, and potentially our lives today. In this article, we are going to clarify what shock waves are, what phase-transforming materials do, and possible opportunities with those materials in the future.

#### The Basics of Waves

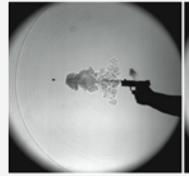
To begin to understand shock waves, let's first consider waves in general. Waves move energy from one location to another location and do not convey the medium where the wave travels. For example, sound can be conveyed through the air, ripples are waves traversing a lake, and light travels through empty space. Shock waves are a particular type of wave, and unlike gentle ripples, shock waves are abrupt, powerful, and strong. For instance, a fast-moving jet breaking the sound barrier or an explosion conveying a blast of energy both create

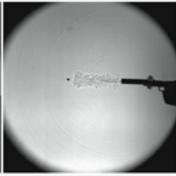


Manoj K.S Research Scholar

shock waves. Shock waves are a type of wave but unlike soft ripples, shock waves are sudden and strong. Think about how a fast-moving jet can break the sound barrier or an explosion sends out a powerful blast both cases create shock waves.

Shock waves are produced when something is traveling faster than the sound in that material. This results in a sharp, almost instantaneous change in pressure, temperature, and density. It's a little like an instantaneous push or hit that causes something to compress very quickly.



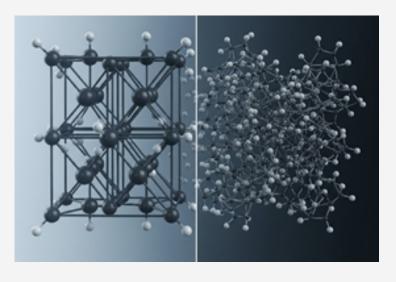


Source: High-speed Imaging of Shock Waves (05.08.2025, 02.38 pm)

For instance when a bullet travels through metal, it creates rippling shock waves that are sent through the metal around the point of impact. These waves causing the atoms inside the metal to become excited and move rapidly and at times could even change the structure of the metal.

#### Phase-Transforming Materials

The materials such as water, metal, or plastic can exist in different phases solid, liquid, gas, or even different types of solids. For example, depending on temperature and pressure, water can be ice, liquid water, and steam. Some materials can rearrange their internal structure even within the solid phase and just switch from one packing of atoms to another without melting. This is called a phase transformation.



Source: Phase Change Materials & Devices, Gao Liu Research Lab, Berkley. (05.08.2025, 04.47 pm)

#### **Phase Transformation Under Shock Waves**

When shock waves migrate through materials that undergo phase transformations, the shock wave can convert the material's atomic structure from an original atomic arrangement to a new atomic arrangement almost instantaneously. For example, a solid metal could go from one solid version to another solid version, which is stronger or tougher, through a shock wave.

This modification could influence the properties of materials such as strength, flexibility or energy absorption. Consider a material that becomes toughened the more it is impacted, or a material that can absorb shocks to protect important equipment or even people. instantaneously. For example, a solid metal could go from one solid version to another solid version, which is stronger or tougher, through a shock wave.

This modification could influence the properties of materials such as strength, flexibility or energy absorption. Consider a material that becomes toughened the more it is impacted, or a material that can absorb shocks to protect important equipment or even people.

#### **Everyday Examples and Uses**

It can be used effectively to assist in Medical Treatments, and to give an example, shock wave therapy is useful in treating kidney stones or healing bone injuries. Shock waves break stones down into smaller pieces or stimulate healing in adjacently soft tissue. In an industrial context, shock waves can assist with processes like forming or cutting metals, where material needs to be formed or modified rapidly. Very importantly, they can also be made to act like Material Products for Safety Equipment Materials. Materials that work and transform on impact would create better helmets, and parts for cars and protective gear that can absorb impact better. Some of the Scientific and Engineering Implications of this work relating to acoustic shock waves are: Materials to create stronger, and lighter, for cars, airplanes, and buildings. Materials that can protect against explosions or impacts by absorbing energy efficiently are also dependent on these shock waves. Improvements of electronics, and machines that have to work in extreme circumstances (i.e. space and deep underwater areas.)

#### **Advanced Materials for Tougher World**

The future is promising, especially for phase-transforming materials influenced by shock waves.

Researchers are working on new alloys and composites that have properties that can be changed on demand with exciting potential. Protective gear that becomes stiff only upon impact. Flexible electronics that can self-heal when damaged. These properties of particular materials under acoustic shock wave loaded conditions could possibly make them a new tougher material for possible use in future applications such as more resistant use in high energy radiation resisting auto crafts for exploratory, expedition type voyages on planets, etc.

Phase-transforming materials can also assist in Energy storage and conversion, where they can enhance batteries and fuel cells, and mitigate waste by technology that is lasting and/or reusable, and impact transportation through lighter and safer vehicles. Space Exploration and Defence. In extreme environments, especially outer space, materials that will withstand rapid shocks due to impact and temperature change are essential. The same is true for defence technology, in particular, where life could be saved with protective Armor that may adapt to a threat.



Source: https://www.flyajetfighter.com (05.08.2025, 12.10 pm)

#### **Challenges and Research Directions**

Despite promising discoveries, working with shock waves and phase-transforming materials is difficult. The processes are fast, so measuring the change requires a great deal of advance preparations. It is inherently difficult to design materials that behave predictably under shock.

Manufacturing these materials in large quantities remains complicated and expensive; however, the work being done and the research continuing in physics, materials science, and engineering is helping to overcome these challenges.

Essentially it will serve as bridging Science and everyday life, the study of shock-waves and phasechange materials shows how cutting edge Science can be applied to use in the real world. The process may begin in high-tech labs but the resultant engineered materials will create safer buildings, safer vehicles or even better medical instruments for us all to use. For their shock response their industries will change, such as the building and construction industry and the transportation industries and defines revolutionized. For example, we could see a rise of earthquake proof buildings or aircrafts that would be able to withstand more impacts. Phasechanging materials can be considered a progression toward "smart" materials - materials that can sense and respond to their environment. These types of materials may lead to products like self-healing materials, self-adaptive Armor, or self-healing sensors. An ability to make materials that react on impact, will give engineers the ability to manufacture products that are significantly safer but lighter and more effective. This is critical in cases where reducing weight is key in the manufacturing process as in electric vehicles and outer space.

#### Conclusion

Shock waves are strong bursts of energy that can fundamentally change the materials they propagate through. When paired with phase-transforming materials - materials that can change their internal structure - the opportunities are exciting for the development of stronger, smarter, more adaptable materials. From medical treatments and safer cars, to energy-efficient devices and space exploration, the future of shock waves and phase-transforming materials is bright and promising. As science progresses, these technologies may just become a part of our daily lives and create a safer and sustainable world for all of us.



### The Need for Clean Energy and Environmental Solutions

we completed our MSc project on the synthesis of nanomaterials for sensor applications. Through this work, we gained a deep understanding on the versatility of nanomaterials and their potential uses. Eventually, we volunteered to organize a workshop on material science, where we learned about the risks of energy-related pollution and the environmental challenges projected beyond 2040. It became clear to me that our research should be directed toward serving society. During our Doctoral study at Thiagarajar College of Engineering for our PhD, we had the opportunity to work on water splitting and dye degradation applications, both of which offer promising solutions to environmental issues. This work has deeply motivated me to contribute meaningfully to sustainable technologies. The 21st century is marked by critical environmental challenges global warming, fossil fuel depletion, and pollution.



Source: H2020 FET projects related to Green Technologies et.al, (5 Aug 2025-2.00 PM)



Pretika PA Research Scholar





P. Ragul & R. Bhuvanesh Kumar Research Scholars

Scientists across the globe are actively developing advanced solutions, and one of the most promising directions is the use of nanomaterials. These materials hold the power to revolutionize.

#### Nanomaterials: Tiny Structures, Massive Impact

Nanomaterials are engineered at the scale of billionths of a meter and exhibit extraordinary properties due to their high surface-area-to-volume ratio and quantum effects.

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These features make them highly efficient in energy generation and environmental remediation.

### **Engineering Smarter Materials: Doping and Morphology Control**

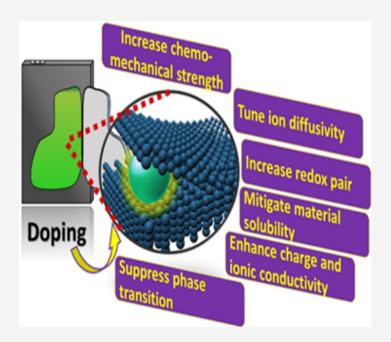
The performance of nanomaterials relies heavily on precise design strategies. Morphology control involves creating structures like hollow spheres, nanosheets, or nanorods that enhance light absorption and charge migration, crucial for improved catalytic efficiency. On the other hand, Doping introducing trace amounts of other elements into the material modifies its electronic structure. Doping helps to extend visible light absorption and promotes better charge separation. For example, nonmetal dopants such as nitrogen, boron, and sulfur create oxygen vacancies or defect states, boosting performance environmental in and energy applications. These strategies enable nanomaterials to respond effectively in areas such as photocatalysis, dye degradation, and water splitting

### Heterojunctions and Hybrid Systems: Synergistic Designs

While individual semiconductors exhibit remarkable properties, they may reach a saturation point in terms of performance when faced with challenges such as fast charge recombination and limited light absorption properties. To address these challenges, researchers have turned their focus towards developing heterojunctions, which are interfaces that form between two different semiconductor materials. Heterojunctions yield internal electric fields that are effective at separating charges such that the electrons and holes will migrate in opposite directions, minimizing the energy lost to recombination. Within heterojunctions, several types exist, such as Type-II, Z-scheme, and S-scheme, all of which are defined by differing energy band alignments and charge transfer mechanisms.

This directional charge transport assists with the overall catalytic efficiency.

An example would be when a wide-bandgap semiconductor, such as TiO<sub>2</sub> or ZnO, is coupled with narrow-bandgap visible-light absorbers, effectively extending the light-absorption range while still taking advantage of the strong oxidizing properties.

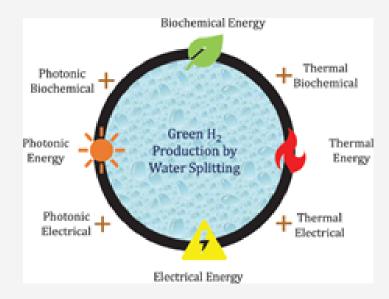


The introduction of conductive materials, like reduced graphene oxide or carbon nanotubes, not improved electron mobility in only the heterogeneous catalyst but also increased the longevity of the system under prolonged use. Hybrid photocatalyst systems were also explored for their versatility as multifunctional hybrid photocatalyst concepts for CO2 reduction to fuels, antibacterial and anti-fog coatings, purification, and solar fuels.

#### Photocatalytic Water Splitting: Fuel from Sunlight

Hydrogen is gaining attention as a clean, zeroemission fuel. Among the methods of hydrogen production, photocatalytic water splitting stands out for its simplicity and sustainability. By mimicking natural photosynthesis, water splits into hydrogen and oxygen using sunlight and a suitable photocatalyst.

The catalyst must absorb visible light, have a suitable bandgap (1.8–3.0 eV), and possess conduction and valence band positions that align with water's redox potentials. Stability under light, resistance to corrosion, and effective charge transport are also key. Metal oxides, doped materials, and layered perovskites have shown promise for this reaction, potentially allowing hydrogen to replace fossil fuels as a primary energy source.



Source: Mohammed Masud Rana et.al, (5 Aug 2025-2.40 PM)

#### From Lab to Society: Bridging the Innovation Gap

While lab-scale results are promising, their real impact lies in practical applications. Key barriers include high costs, synthesis scalability, and long-term stability. Fortunately, many nanomaterials can be synthesized using green chemistry, which employs water-based solvents, low temperatures, and abundant resources—reducing environmental impact and supporting large-scale production. Photocatalytic systems also offer flexibility, as they can be used in decentralized applications such as water purification, solar hydrogen generation, and air cleaning, especially in remote or underserved areas.



Source: Impact Investing meets Real Estate et al, (5 Aug 2025-2.50 PM)

#### A Vision for a Cleaner Future

Nanotechnology is paving the way to tackle some of humanity's greatest challenges. **Nanomaterials** are already forming backbone of systems that purify water, clean air, generate renewable energy. and Their applications now span energy, agriculture, environment, and even healthcare. The journey to a sustainable future won't be marked by one invention, but by a multitude of innovations across fields.

With smarter design, data-driven approaches, and green chemistry, nanomaterials can achieve transformative results. Dreams of using sunlight to produce clean fuel, purify water, or develop decentralized, affordable energy systems are becoming reality. These small-scale materials carry large-scale promise. With more research, responsible development, and equitable access, we can build a future where sustainability is standard, not exceptional.

There's something profoundly humbling about looking up at the sky. When it's vast and empty, it offers a quiet kind of beauty. But when night falls and stars begin to scatter across the darkness, the sky transforms into a mesmerizing canvas -timeless, infinite, and alive. For me, this wasn't just a scene to admire; it became a portal to wonder. I have always believed that the sky is a kind of magic and physics "The unseen hand guiding its marvels". It is the magician behind the curtain. Every time I gaze upward, I feel a sense of awe that words can barely capture. From the cataclysmic birth of the universe in the Big Bang to the enigmatic pull of black holes, the cosmos has never failed to stir something deep within me. It was through this lens of awe and curiosity that I began to see time not as something we move through, but as something far more profound - a dimension as real as length, width, and height. And in that realization, a journey began.

In physics, the idea of time as the fourth dimension has fundamentally changed how we view the universe. While we move through three familiar dimensions - length, width, and height - time expands our understanding into a four-dimensional fabric called spacetime. This idea, made famous by Albert Einstein's theory of relativity, provides the scientific basis for key themes explored in the movie Interstellar. In this article, we explore the physical meaning of time as the fourth dimension and how Interstellar brings this abstract concept to life.

#### The Birth of Four-Dimensional Spacetime

Traditionally, space was viewed as an unchanging, absolute backdrop where events took place. However, Einstein's relativity transformed this view by combining space and time into a single, interconnected concept called spacetime.





S. Hemapriya & M. Deepikaa Research Scholars

In this model, each event is described by four coordinates: three spatial (x, y, z) and one temporal (t).

#### **Key Principles:**

Time is not absolute: It can pass at different rates for various observers, depending on their velocity and gravitational field.

Events in spacetime: Rather than happening just "here" or "there," all events exist within a four-dimensional coordinate system.

Einstein described the universe as a massive, four-dimensional "block" where all events-past, present, and future-coexist within the fabric of spacetime. Time becomes another axis, similar to length, width, or height, but with properties that set it apart from spatial dimensions, such as having an inherent "arrow" pointing from past to future. Christopher Nolan's Interstellar explores the idea of time as a dimension, especially in its depiction of time dilation-the phenomenon where time passes at different rates depending on gravity and speed. This concept is directly based on Einstein's general theory of relativity.

Time Dilation by Gravity: In Interstellar, astronauts exploring a planet near a black hole experience time much more slowly than people far from it. For every hour they spend on the earth, years pass elsewhere in the universe.

Wormholes as Tunnels Through Spacetime: The protagonists use a wormhole - a theoretical shortcut through spacetime - to travel to distant galaxies, visually illustrating how the dimensions of space (and possibly time) can be bent or folded by gravity.

The film's famous "bookshelf scene" takes this abstraction further.

Cooper, the protagonist, finds himself in a tesseract-a four-dimensional construct-where he can perceive and potentially influence points along the time axis, much like one can move up and down, left and right. An artistic rendering of a wormhole illustrating how it connects two distant points in spacetime, folding the fabric of the universe. Here's what physics tells us about experiencing time as a dimension.

#### The Arrow of Time:

While we can move freely in the three spatial dimensions, we inexorably move forward in time. This is due to the second law of thermodynamics, which implies an increase in entropy (disorder) and gives time its perceived direction of flow.

Worldlines: In spacetime diagrams, each object traces a "worldline" that shows its movement through space and time. Crossing worldlines is seen as the intersection of different events.

#### The Mystery of the Fourth Dimension

Unlike our experience with space, traveling backward or sideways in time remains theoretically and technologically impossible, even though it is mathematically possible according to Einstein's equations.





Time travel, paradoxes, and causality are intensely debated issues in modern physics.

#### **Black Holes and the Theory of Time**

In modern physics, black holes are more than just mysterious cosmic objects - they are laboratories for testing the most profound ideas about space and time. At the heart of this connection is Einstein's theory of general relativity, which shows that mass and energy warp the fabric of spacetime. Black holes, with their immense mass concentrated in an infinitesimally small region, distort time itself in extreme ways. Exploring how black holes influence time can transform our view of the universe.

#### Time in Einstein's Theory of General Relativity

In Newtonian physics, time is absolute-it ticks the same for everyone, everywhere. In Einstein's general relativity, time is relative and depends mainly on two factors: the velocity of the observer (Special Relativity) and the strength of the gravitational field (General Relativity). Einstein demonstrated that gravity is not a force but a curvature of spacetime caused by mass. Time moves more slowly in stronger gravitational fields-a phenomenon known as gravitational time dilation.



force but a curvature of spacetime caused by mass. Time moves more slowly in stronger gravitational fields-a phenomenon known as gravitational time dilation.

#### **Extreme Gravity & Time Dilation**

A black hole is a region in space where gravity is so strong that nothing, not even light, can escape. It contains a singularity at the centre-a point where mass is infinitely dense and spacetime curvature becomes infinite. The event horizon is the boundary around the black hole from which nothing can escape. The singularity is the core point of infinite density. And the accretion disk is a disk of matter spiralling into the black hole.

#### Time Near a Black Hole

As you approach the event horizon, time slows down relative to a distant observer. To someone far away, a clock near the black hole seems to tick more and more slowly. At the event horizon, time appears to stop from the perspective of an external observer. This explains why black holes trap matter; they don't just trap matter, they also slow and distort time itself experimental Evidence of Gravitational Time Dilation.

#### 1. Hafele-Keating Experiment (1971):

Because of the high speed and reduced gravity at altitude, atomic clocks on airplanes gained time in this experiment when compared to ground clocks.

#### 2. Pound-Rebka Experiment (1959, 1964):

By measuring gamma-ray redshift at various elevations, these experiments verified gravitational time dilation; the 1964 refinement matched general relativity to within 1% accuracy.

#### 3. Gravity Probe A (1976):

This experiment involved sending a hydrogen maser clock on a rocket to a high altitude.

By comparing the rocket-based clock with one on Earth, scientists confirmed that time moves faster in weaker gravitational fields. The experiment validated the predictions of general relativity with an impressive accuracy of 0.01%.

In Interstellar, the crew visits Miller's Planet, which is near the supermassive black hole Gargantua. Due to intense gravity, time moves extremely slowly there, with 1 hour on the planet equalling 7 years on Earth. When Cooper and his team return, decades have passed for others, even though only hours have elapsed for them. While dramatized, this effect is scientifically accurate, assuming a large enough black hole with a slow spin and the right orbiting conditions. Time is not universal; it is influenced by gravity and motion. The past, present, and future are not absolute; they vary for each observer depending on their position and movement. Spacetime is dynamic, and black holes are locations were, from particular perspectives, time can essentially "pause." Some physicists even suggest that inside the event horizon, the roles of space and time might making time resemble a spatial switch, dimension. Black holes serve as the strongest demonstration that time is a dimension, not fixed but relative and adaptable. Their immense gravity bends spacetime so intensely that time can nearly come to a stop near them. This isn't just theoretical; it has been observed, modelled, and explained through Einstein's profound insights. By studying black holes, physicists are not only investigating exotic objects in space but also probing the very fabric of time itself.

#### Reflections from "Interstellar"

By presenting time as the fourth dimension, both modern physics and Interstellar invite us to rethink our assumptions about the universe. In the end, "love transcends dimensions," as the film poetically suggests, but it is our scientific understanding of those dimensions, including time, that expands our grasp of the cosmos.

# Turning Heat into Power: The Promise of Thermoelectric Heusler Alloys

HEAT

#### **Introduction:**

Turning wasted heat into clean power is a really cool idea, especially since we need more energy but don't want all the pollution. Thermoelectric Heusler alloys could be a great way to do this because they have special properties we can adjust. I became interested in this because numerous sources of heat are wasted by factories, vehicles, and various household appliances. If we could grab some of that heat and reuse it, our energy systems would work way better. I want to not just learn new things but also make stuff that helps us have a more sustainable future.



Source: MIT News Office (05.08.2025, 10.24 am)

This research looks at these Heusler alloys to try to make new materials that are good at turning heat into power. If we get this right, we could use less fuel, make less pollution, and have energy sources that are more local. Turning waste heat into clean energy could really help society. For many years, Heusler alloys were mostly known for their magnetic abilities and their role



Nandhakumar Murugan Research Scholar

in spintronics (a branch of electronics that uses the spin of electrons). But recently, scientists have discovered that these same alloys can also work surprisingly well as thermoelectric materials. This opens up the exciting possibility of using them to capture waste heat from car engines, factories, and even our own bodies and turn it directly into useful electricity on a large scale.

#### What Makes a Material Thermoelectric?

Thermoelectric materials rely on a principle called the Seebeck effect. When one side of a material is hotter than the other, electrons drift from hot to cold, creating a voltage. The stronger the effect, the more power we get. Most materials that conduct electricity well also conduct heat too easily causing the temperature difference (and power generation) to disappear. Heusler alloys break this trade-off beautifully. Due of their extreme atomic structures, we can change their composition to conduct electrons without losing heat.

Heuslers and full-Heuslers, each based on different ratios of metals like nickel, cobalt, titanium, tin, or antimony. By carefully swapping atoms within their crystal lattices, scientists can control their electronic structure like knobs on a control panel enhancing the Seebeck coefficient, lowering thermal conductivity, and ultimately enhancing thermoelectric performance. One family in particular half-Heusler compounds such as TiNiSn has shown impressive efficiency at mid-to-high temperatures, where most industrial waste heat lives.

#### **Emerging Real-World Applications**

#### • Automotive Waste-Heat Harvesting

Modern cars lose ~70% of fuel energy as heat through exhaust gases. Thermoelectric Heusler modules embedded in the exhaust system could convert that heat back into electricity to power onboard electronics improving fuel efficiency.

#### • Wearable Power Generators

Lightweight, non-toxic Heusler materials are being explored for body-heat–powered wearables, potentially charging small sensors and fitness trackers continuously without batteries.

#### • Automotive Exhaust Recovery

Car and truck engines waste most of their fuel energy as heat. Heusler-based thermoelectric modules placed in the exhaust system can turn that heat into electricity to run onboard electronics, increasing overall fuel efficiency.

#### • Remote Sensors & IoT Devices

In places where changing batteries is difficult like oil pipelines or wildlife tracking stations Heusler thermoelectric generators can use simple temperature differences (day vs night, underground vs surface) to power sensors year-round.

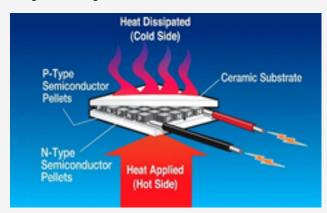
#### • Industrial Heat Recovery

Factories, power plants, and steel mills produce enormous amounts of residual heat. Solid-state Heusler-based thermoelectric generators can sit silently alongside machinery, feeding captured energy back into the grid.

Fast Facts: Heusler Alloys at a Glance

Feature	Advantage
Crystal structure	Highly tunable electronic properties
Thermal conductivity	Naturally low
Environmental impact	Often less toxic than alternatives
Operating temperature	300–900 K (ideal for waste-heat)
Major compound examples	TiNiSn, ZrNiSn, NbFeSb
Key Applications	Spacecraft power systems, Radioisotope

#### **Graphical Representation**



Source: MIT News Office (05.08.2025, 10.55 am)

#### What's Next? From Lab to Life

Although engineers have already demonstrated Heusler thermoelectric modules in prototype vehicles and power generators, arge-scale manufacturing remains a hurdle. Researchers currently optimizing are inexpensive synthesis techniques, like spark plasma sintering and 3D printing, to make in bulk without these allovs losing performance.

#### A Future That Runs on Waste

If successful, thermoelectric Heusler alloys could lead to a world where energy recycling is as common as trash recycling turning hot engines, industrial furnaces, and even our own body heat into meaningful sources of clean electricity.



#### SUCCESS

## How to Succeed in Physics: Study Hacks from Top Students



We all know that the king of science is none other than PHYSICS. Why is it the king? Because it provides the foundation for all other disciplines. Is physics really hard? The answer is NO. Let me explain in this article how physics can be easy to understand. In this article, you'll gain clarity on why most students feel physics is tough, how to learn physics in the easiest way, and some helpful study tips. Let's start with a key point: Physics is not tough. The main reason many students find it difficult is due to a lack of basic knowledge in the subject. Where do you get this basic knowledge? From grades 6 to 11. All the core concepts remain the same across these grades. For example, from 6th standard to 11th standard, you'll come across "MEASUREMENT, FORCE. chapters like: ATOMS, LIGHT, SOUND," etc.

These chapters contain the foundational concepts of physics. If you build a strong foundation in them, you can learn physics easily, peacefully, and joyfully. Some students may feel that Classical Physics is difficult because it involves MECHANICS, THERMODYNAMICS, KINETIC THEORY, and a lot of MATHEMATICAL **CALCULATIONS.** So how do we overcome this? It's a simple process just understand the concept. Now you may ask: how can I understand the concepts? The answer is: go back and study the lower-grade books starting from the 6th standard, without any ego  $\odot$ . After learning the concept, try to connect it with real-life applications. Talk to yourself don't worry about your surroundings and feel the subject.



Sivaprakash B.E. Mechanical Enggineering.

Since physics is the study of nature, you can observe it in practical applications around you. For example, ask questions like: why do vegetables boil faster when you add a pinch of salt? What happens to the boiling point? Once you deeply understand the concepts, go through the derivations and clarify any doubts with your friends, the internet, or your teachers. Should we study physics daily? Yes! You should allocate just 30 minutes to 1 hour per day. If you struggle with MODERN PHYSICS, read about the history behind the discoveries and the scientists involved. It will motivate you to read the entire chapter.o learn anything, the first thing you need is self-discipline and self-confidence.

- Learn basics from the lower grade books (From 6th standard).
- Observe the concepts in real life. (From Kitchen to Rocket).
- Deal with the derivation part in Classical Physics and clarify the doubts (since which contain more numericals)
- Read the history behind every innovation to make yourself curious about PHYSICS.



#### Introduction

Whether it's the crack of a bat or the leap of an athlete, sports are where physics comes alive in full motion. Many of us enjoy the thrill of watching a ball swing through the air or a jumper fly across a sandpit, but behind those moments are elegant laws of nature at play. This article explores how physics powers two popular sporting actions fast bowling in cricket and the long jump in athletics.

#### Fast Bowling: Mastery of Motion and Air

Have you ever wondered how some bowlers make the ball 'talk' in the air? Fast bowling isn't just a feat of athleticism it's a calculated use of physics that begins from the moment the bowler takes their first step.

#### 1. Momentum and Energy Transfer

The run-up is not just for show. It's where bowlers store energy. When they sprint toward the crease, they generate linear momentum, which they pass on to the ball through a complex chain of body movements. The longer and smoother the run-up, the more effective the energy transfer. Legendary pacers like Shoaib Akhtar, Brett Lee, Shane Bond often reached above 150 km/h by mastering this transition.

#### **Physics in Action:**

Momentum = mass × velocity Energy =  $\frac{1}{2}$  × mass × velocity<sup>2</sup>

#### 2. Arm Whip and Angular Speed

Beyond the legs, it's the arm that really finishes the job. The shoulder acts like a pivot point while the arm acts like a whip. This rotation creates angular velocity, increasing the ball's final speed.

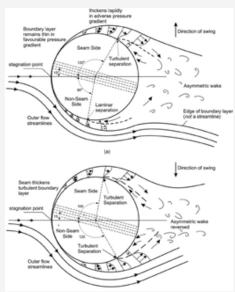


S. Kamalesh
III year,
B.E. Mechanical Engineering,

A snappy wrist flick can add the final punch. It's almost poetic—force, form, and fluid motion all in sync.

#### 3. The Science of Swing

Now comes the magical part swing. If one side of the ball is shiny and the other is rough, air moves faster over the smooth surface, creating pressure differences. The ball moves or 'swings' towards the low-pressure side.



Source: ResearchGate - Bharat Patil et al.

The seam further disrupts airflow, enhancing this effect. This is known as the Magnus effect, which adds curve when the ball spins.

O-AATRAL-2025 2'

Real-World Example: James Anderson and Bhuvneshwar Kumar make the ball dance in mid-air with these principles. It's less about magic and more about masterful use of air resistance. The given picture describes the airflow comparison between the conventional and reverse swing. Comparison of airflow and boundary layer separation in conventional (top) and reverse swing (bottom). In reverse swing, the turbulent flow separates later on the rougher side, creating a pressure imbalance that curves the ball in the opposite direction.

#### 4. Interesting Facts behind the Reverse Swing

Reverse swing is where physics takes an even more mysterious turn. It occurs when the ball is older, and both sides become rough but one side is still slightly smoother due to polishing. At high speeds (above ~135 km/h), the turbulent airflow dominates both sides, but the side with slightly more roughness creates greater drag, flipping the swing direction opposite to what the batter expects. It's as if the ball is defying intuition curving the "wrong" way, late in the air, with almost no visible change in action. What makes reverse swing truly beautiful is its deceptiveness. The bowler appears to bowl a standard delivery, but due to the fine balance of air pressure, ball condition, and seam angle, the ball suddenly veers in or out just before reaching the batter leaving even the best stunned.

Real-World Example: How Wasim Akram or Dale Steyn use reverse swing in the death overs it's pure science, disguised as sorcery. Long Jump: Physics of Flying Feet- In long jump, every second counts literally. You have a 40-meter runway, one shot at the take-off board, and less than a second of flight. It's the athlete's moment to become a human projectile, and physics makes or breaks that jump.

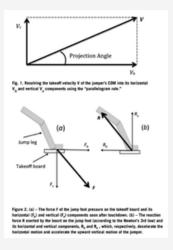
#### 1. Speed Breeds Distance

As the jumper sprints toward the board, they're building kinetic energy. The faster the approach, the more energy is available for the jump.

**2.** Take-off Angle: Not Too High, Not Too Low Unlike what textbooks tell us about ideal projectile

motion (45°), long jumpers need a shallower take-off about 20° to 22°. Why? Because air time doesn't win gold—distance does. A steeper angle gives more height, but less forward travel. So they aim low, fly forward, and land clean. Physics Tip: Range (R) =  $(v^2 \times \sin 2\theta)$  / g Where g = 9.81 m/s<sup>2</sup>3.

In-Air Technique and the Landing Trick. Once airborne, it's about posture. Athletes swing their arms and cycle their legs mid-air not to look fancy but to stabilize their center of mass. This helps them stay in control. During landing, they throw their feet forward and lean their torso to avoid falling backward. Sometimes, those final 10 cm make all the difference.



These pictures illustrate the three segments of a jump take-off distance  $(L_1)$ , flight distance  $(L_2)$ , and landing distance  $(L_3)$  with the parabolic path of the jumper's centre of mass. And also shows the decomposition of the centre-of-mass velocity into horizontal  $(V_h)$  and vertical  $(V_v)$  components essential for understanding how take-off angle and run-up speed affect total distance.

#### Conclusion

In essence, physics is the hidden force behind athletic brilliance. From the parabolic arc of a long jumper to the reverse swing of a cricket ball, it's all about motion, force, and timing. Athletes may not always realize it, but every stride, leap, and spin are the live demonstration of scientific principles. It's this blend of skill and science that makes sports not just thrilling to watch—but fascinating to understand.

# TORCH BEARERS OF THE DEPARTMENT



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# RESEARCH SPECIALIZATION

Smart Materials|| Quantum Computing

### **PUBLICATION STATISTICS**

(as of July-2025)

Total Number of Publications – 135 || Seminars and conferences Organized - 32 || Ph.D's Produced – 18||Invited Talks given - 65||Guest Lectures -150||Projects completed- 09|| Citations – 1616 || h-index – 18||i-10 index- 35

# Dr. M. Mahendran, Ph.D, FASCh, PDF.,

Dr. M. Mahendran is Professor and Head of Department of Physics at Thiagarajar College of Engineering, Madurai. He has been working at Thiagarajar college of Engineering since 1997. His fields of research is on smart materials and Quantum computing. Dr. Mahendran completed his Ph.D at Madurai Kamaraj University and did two postdocs at Weizmann Israel, Okayama University, Japan under JSPS fellowship and at BOYSCAST Massacheusetts Institute of Technology, America. He has more than 135 publications and has produced 18 ph.D.

He has acted as principal investigator for around nine prestigious projects. He has acted as a resource person and has given 65 invited talks. He has given more than 150 guest lecturers. Apart from this he acted as a visiting Research Scholar at university of Barcelona, spain, visiting Associate professor at Tohoku university, Japan. He is a member of National Advisory committee, Magnetic society of India, Board of studies Anna university, Chennai and chairman of Magnetic society of India. He received various grants from CSIR, ISRO,DRDO, DST, UGC and SERB.

He has organized various seminars, conferences and workshops. He is acting as a member of various societies such as Institute of smart structures and systems, Indian society of Technical education, Indian Physics association, Institute of association of physics teachers, Institute of Electrical and electronic Engineers and The American nano society. He is a highly enthusiastic person who is active in conducting various programs and thereby striving for the growth of the department in all dimensions. Through his proactive efforts he created a vibrant environment that inspires innovation and continuous improvement.

#### **List of Few Publications**

- 1. P. Sundararajaperumal, M. Mahendran, P. Velusamy, Ikhyun Kim, Surfaces and Interfaces, 65, 2025, 106410.
- 2. S.R. Sagitha, V. Aravindan, M. Mahendran, M.N. Kumar, Applied Physics A, 131 (4), 2025, 333.
- 3. V. Aravindan, V. Vijayanarayanan, B. Karuppasamy, K. Sakthipandi, M. Mahendran, Materials Today Communications, 2024, 39,108599.
- 4. P. Sundararajaperumal, P. Velusamy, M. Mahendran, IEEE, 2024, 1-2.
- 5. Aravindan, AK Rajarajan, V. Vijayanarayanan, M. Mahendran, Physica B: Condensed Matter, 2022, 647: 414370.

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O-AATRAL-2025



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#### RESEARCHSPECIALIZATION

Vacuum Science || Thin Film Technology || Electrochromism || Transparent Electronics || Quantum Computation ||

# **PUBLICATION STATISTICS**

(As of July-2025)

Total Number of Publications 10 h-index -10 Citations -712

# Dr. A. Karuppasamy, Ph.D, PDF.,

Dr. A. Karuppasamy is a doctorate from Indian Institute of Technology Madras (IITM), Chennai and a post doctorate from Fraunhofer Institute for Electron and Plasma Technology, Dresden, Germany and Technical University of Dresden, Germany. He has 25 years of teaching cum research experience and has rendered his service under various capacities in institutes like IITDelhi, IITMadras, Madura College and PSNA

College of Engineering and Technology. Currently, he is working as an Assistant Professor in the department of Physics, Thiagarajar College of Engineering, Madurai.

His area of expertise includes, thin film devices, vacuum technologies, electrochromics, photocatalysis, nano and quantum materials. He has published research papers and conference papers in reputed journals and has a book chapter and patent (filed) to his credit.

He has delivered lectures on popular science topics in schools, colleges and research forums in India, Germany, USA and Switzerland. He is an active life member in professional societies like ISTE and IAPT.

#### **List of few Publications**

- 1. A. Karuppasamy, Materials Chemistry and Physics, 301, 2023, 127580.
- 2. A. Karuppasamy, Applied Surface Science, 359, 2015, 841.
- 3. A. Karuppasamy, Applied Surface Science, 282, 2013, 77.
- 4. A. Karuppasamy and A. Subrahmanyam, Journal of Applied Physics, 101, 2007, 6.
- 5. A. Subrahmanyam and A. Karuppasamy, Solar Energy Materials and Solar cell, 91, 2007, 266.

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Supercapacitors & Batteries|| Photoelectrochemical (PEC) Water Splitting || Chemical & Physical

Deposition Techniques || Doped Metal Oxides || Dye Degradation & Wastewater Treatment || Gas Sensors & Optoelectronic Devices

### **PUBLICATIONS STATISTICS**

Total number of publications: 35 || HIndex:18 || i-10 index: 24 || Conference Paper:10 || Best Paper: 1 || As a Reviewer: 85 || Workshop: 10 || Conference Attended:30

# Dr. P. Velusamy, Ph.D, PDF.,

Dr. Velusamy is working as an Assistant Professor at Thiagarajar College of Engineering, Madurai, he completed his doctoral research on Transparent Conducting Oxide Thin Films for Solar Cell and Gas Sensor Applications at Bharathidasan University. My Ph.D. work focused on the synthesis, characterization, and functional analysis of TCO thin films tailored for optoelectronic and gas sensing applications.

His current work focus is on sustainable hydrogen energy production and storage. With over 15 years of experience, he has published over 30 research articles in international journals and 8 more is under review.

He did postdoctoral research at Henan University, SSN Research Center, and Yan'an University, focusing photocatalytic, electrocatalytic, photoelectrochemical water splitting applications. He currently serve as an Assistant Professor at Thiagarajar College of Engineering, Madurai, focusing on sustainable hydrogen energy production and storage. Their research expertise includes nanomaterials development, thin film deposition techniques, materials characterization, device fabrication, carbon-based materials, and independent project handling. The longterm vision of his research group is to contribute to affordable and sustainable nanomaterial-based energy solutions for a greener future.

# **List of few Publications**

- 1.P. Velusamy, Shanhu Liu, M Sathiya, Awais Ahmad et.al. ACS Appl. Nano Mater, 7(5), 4707–4720.
- 2.P. Velusamy et.al. Chemosphere, Volume 329, 2023, 138535.
- 3.P. Velusamy et.al., Chemosphere, Volume 321, 2023, 138007.
- 4.P. Velusamy, R Ramesh Babu, Awais Ahmad et. al., ACS Omega, 7(39), 2022, 35191-35203.
- 5.P. Velusamy. et. al., Diamond and Related Materials, Volume 157, August 2025, 112489

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Crystal Growth || X- Ray Crystallography||
Biological Applications ||
NLO Materials || Nano – Materials for
Energy and Environmental
Applications

# **PUBLICATION STATISTICS**

(As of July-2025)

Total Number of Publications – 11 || Best Poster's – 2 || Conferences / School and Workshops – 24 || Citations – 59 || h-index – 5

# Dr. M. Tamilelakkiya, Ph.D.,

Dr. M. Tamilelakkiya is currently working as an Assistant Professor in the Department of Physics at Thiagarajar College of Engineering, Madurai. She holds a strong academic foundation in Physics, having completed her undergraduate and postgraduate degrees from Lady Doak College in 2010 and 2012, respectively. She went on to pursue her M.Phil. in Physics from Madurai Kamaraj University in 2013 and earned her Ph.D. in Physics from the same university in 2019. Dr. M. Tamilelakkiya has previously held academic positions at various colleges.

Her doctoral research centered on the growth of single crystals tailored for biomedical application. Presently, her research interests encompass the growth of functional crystals for nonlinear optical (NLO) applications and the synthesis of nanostructured materials for energy-related devices. She is also actively engaged in collaborative research and encourages academic exchange, providing guidance and infrastructure support to students from neighboring institutions for internships and project work. With a balanced focus on both teaching and research, Dr. M. Tamilelakkiya remains dedicated to advancing materials science through crystal engineering and nanotechnology, aiming to address emerging challenges in energy, environmental and biomedical domains.

#### List of few Publications

- 1. Vinola Johnson, Thiyagarajan Maadhu b, M. Tamilelakkiya et al, Inorganic Chemistry Communications 178, 2025, 114629.
- 2. M. Tamilelakkiya et al, Journal of Nano-Structures & Nano-Objects, 40, 2024,101338.
- 3. K. Anitha, M. Subha, M. Tamil Elakkiya et al, Journal of molecular structure, 1244, 2021, 130850.
- 4. P. Justin, M. Tamilelakkiya, A. Mythili, P. Velusamy et al, Journal of Materials Science: Materials in Electronics, 30 ,2019) 16207–16215.
- 5. K. Anitha, M. Subha, M. Tamil Elakkiya M. Tamilelakkiya et al, Journal of molecular structure, 1173 (2018) 635-646.

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#### RESEARCH SPECIALIZATION

Li-ion Batteries || Polymer Electrolytes || Solid-State Ionics || Cathode Materials || Nanomaterials || Supercapacitors

# **PUBLICATION STATISTICS**

(As of July 2025)

Total Number of Publications – 19 || Conferences / School and Workshops – 10|| Citations – 265 || h-index – 9

# Dr. S. Karthickprabhu, Ph.D.,

Dr. S. Karthickprabhu is a committed academician and researcher specializing in energy materials and lithium-ion battery technologies. Holding a Ph.D. in Physics from Kalasalingam University, his research has mainly centered on lithium-ion batteries, especially olivine-based cathode materials and polymer electrolytes, contributing to innovative energy storage solutions. He has published over 19 research articles in reputable international journals such as Journal of Alloys and Compounds, Ionics, Applied Surface Science, and Journal of Power Sources, demonstrating his expertise structural. the electrochemical, and conductivity aspects of battery materials.

Dr. Karthickprabhu's academic career is distinguished by excellence, being a Gold Medalist in both B.sc. and M.sc. Physics. His career includes significant teaching and research roles at institutions such as Kalasalingam University, Sri Kaliswari College, and presently at Thiagarajar College of Engineering (TCE), Madurai, where he serves as an Assistant Professor in the Department of Physics. He has been recognized for his teaching effectiveness by consistently achieving 100% results in Anna University examinations for Engineering Physics courses. Furthermore, his research achievements acknowledged through fellowships like the Junior and Senior Research Fellowships from the Board of Research in Nuclear Sciences (BRNS), Government of India. In addition to his publications, he has actively participated in numerous national and international conferences, presenting his research on advanced materials and energy storage systems. As an esteemed research supervisor under Anna University, he continues to guide students in cutting-edge materials research.

### **List of few Publications**

- S. Karthickprabhu et al, Journal of Power Sources, Volume 648, 2025, 237378.
- G.Hirankumar, S.Karthickprabhu, R.S.Daries Bella et al, Journal of Alloys and Compounds, 548, 2013, 65-69.
- S. Karthickprabhu, G.Hirankumar, A.Maheswaran, C.Sanjeeviraja, R.S.Daries Bella et al, Ionics, 21, 2014, 345-357
- S. Karthickprabhu, K. Karuppasamy, Dhanasekaran Vikraman, K. Prasannaet al, Applied Surface Science, 449, 2018, 435–444
- S. Karthickprabhu, Dhanasekaran Vikraman, A.Kathalingam, K.Prasanna, Hyun-Seok Kim et al, Materials Letters, 237, 2019, 224-227

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First-Principles Materials Modeling || Heusler & High-Entropy Alloys || Machine Learning for Materials Discovery || Spintronics & Thermoelectrics || Perovskite || Hydrogen Storage Materials || Computational Photovoltaics

### **PUBLICATION STATISTICS**

(As of July-2025)

Total Number of Publications – 20 || Best Poster's – 2 || Conferences / School and Workshops – 34 || Citations – 173 || h-index – 8

# Dr. V. Aravindan, Ph.D, PDF.,

Dr. V. Aravindan is an Assistant Professor in the Faculty of Physics at Thiagarajar College of Engineering (TCE), Madurai, where he is engaged in teaching, research, and student mentorship. He earned his Ph.D. in Physics from Anna University, with his research carried out at TCE, focusing on first-principles investigations of electronic structure and physical properties of equiatomic quaternary Heusler alloys for spintronic applications.

The academic journey of Dr. Aravindan began with a B.Sc. and M.Sc. in Physics from The American College, Madurai. He has a strong foundation in theoretical and computational physics, further strengthened by research engagements at prestigious institutions like the S.N. Bose National Centre for Basic Sciences, Kolkata (as a Postdoctoral researcher) and Bhabha Atomic Research Centre (BARC), Mumbai (as a Project fellow).

He primarily focuses his research on first-principles calculations, machine learning for materials discovery, high-entropy materials. and perovskites, with applications spanning spintronics, thermoelectrics, photovoltaics, and hydrogen storage. He has published over 20 research papers in reputed international journals and holds an H-index/i-index of 8. He has actively contributed to numerous national and international conferences, and his work has been recognized with multiple Best Paper Awards. He is a life member of both the Indian Association of Physics Teachers (IAPT) and the Materials Research Society of India (MRSI), and he serves as a peer reviewer for several international journals published by Elsevier and IOP Publishing.

#### **List of few Publications**

- 1. Kumar, M.N., ARAVINDAN, V., Laihnuna, N. and Mahendran, M, Journal of Rare Earths, 2025, DOI: 10.1016/j.mtcomm.2024.108599.
- 2. V. Aravindan, Vijayanarayanan, V., Karuppasamy, B et al, Materials Today Communications, 2024, 39:108599.
- 3. Djamel, B., ARAVINDAN, V., Haidar, E. A., Pachuau, Z., Lalbiakkimaet al, Journal of Physics and Chemistry of Solids, 2024, 195, 112291.
- 4. V. Aravindan, Rajarajan, A. K., Vijayanarayanan, V., & Mahendran, M., Materials Science in Semiconductor Processing,, 2022, 150: 106909.
- 5. V. Aravindan Rajarajan, A. K., Vijayanarayanan, V., & Mahendran, M.et al, Physica B: Condensed Matter, 2022, 647: 414370.



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Thin Films Coatings/Devices || Multi-Functional Materials Research || Ion Beam Technologies || Materials/Device Simulations (COMSOL, SCAPS, RSD, SiMTra)

# **PUBLICATION STATISTICS**

(As of July-2025)

Total Number of Publications - 6 || Patent - 1 || Conference/Workshops - 35 || Citations - 12 || h-index - 2

# Dr. P. Sivakumar, Ph.D.,

Dr. P. Sivakumar is working as an Assistant Professor in the Department of Physics at Thiagarajar College of Engineering. He has a teaching experience of about two years as an Assistant professor in various colleges, and he is interested in both teaching and research. He completed his Ph.D. in Physics from Bharathiar University, Coimbatore, and attained postdoctoral experience in industry (Titan Watch Company). He brings a strong foundation in advanced research and practical application. His academic journey includes serving as an Assistant Professor at KIT- Kalaignar Karunanidhi Institute of Technology, as well as significant research roles during his Ph.D., such as JRF and SRF in DST-SERB-funded projects and Research Fellow under the RUSA 2.0 BEICH Project. In addition to his research expertise, he has developed teaching skills through positions as a PG Teaching Assistant at AKN School, Avinashi, and Guest Faculty at Tagore College of Arts and Science, Puducherry. His technical proficiency was further enhanced during his tenure as a Technical Assistant at Pondicherry University. Collectively, these experiences have equipped him with a comprehensive skill set in experimental physics, research project management, and academic instruction, allowing him to bridge the gap fundamental science between and practical implementation. As an experimental physicist, he has extensive experience in preparing a range of nano to quantum materials, thin film preparation, and coatings on both conductive and nonconductive substrates using multiple thin film coating techniques. He has hands-on experience in various characterization techniques such as FTIR, Raman spectroscopy, AFM, XRD, SEM, TEM, RBS, and Electrochemistry. At present, his areas of research interest lie in the preparation of novel functional catalytic materials for hydrogen production and energy solutions.

# **List of few Publications**

- 1. P. Sivakumar, P. Peranantham, V. V. Sivakumaret al., Nuclear Inst. And Methods in Physics Research, B 534, 2023 1-10.
- 2. P. Sivakumar et al., J. Mater. Sci: Mater. Electronics, 2021, 8767-8777.
- 3. P. Sivakumar et al., Thin Solid Films, 2021, 736, 138917.
- 4. P. Sivakumar et al., J. Vac. Sci. Technol. A, 2020, 38, 063404.

**Indian Patent -** IN Patent 465058 – Synthesis of sub-10 nm zinc tin phosphide ternary semiconductor nanoparticles and chemical method thereof.



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2D Materials || Quantum Transport || Density Functional Theory

#### **PUBLICATION STATISTICS**

(As of July-2025)

Total Number of Publications – 16 || Best Poster's – 1 || Conferences / School and Workshops – 9|| Citations – 99 || h-index – 6

# Dr. A. Santhia Carmel, Ph. D, PDF.,

Dr. Santhia Carmel is currently working as Assistant Professor-Research Faculty in Thiagarajar College of Engineering at Department of Physics. She is a dedicated research faculty member specializing in nanoelectronics, semiconductor device modeling, and 2D materials. With a **Nanoelectronics** from SASTRA Ph.D. Deemed University. academic journey reflects deep commitment to advancing nanoscale device technologies through rigorous theoretical and computational approaches. Her postdoctoral tenure at IIT Gandhinagar focused on reducing contact resistance in Metal-WS, interfaces, contributing to the development of high-performance 2D contact systems. Dr. Carmel's research portfolio includes extensive work on phosphorene nanoribbons, exploring their electronic, optical, and transport properties using Density Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) methods. Her publications in high-impact journals such as Journal of Applied Physics, Physica E, and PCCP demonstrate her expertise in bandgap engineering, negative differential resistance, and device-level simulations. She is proficient in advanced simulation tools including QuantumATK, VASP, and MATLAB, and has contributed to international conferences across Asia, presenting her work on nanoscale devices and 2D materials. Her interdisciplinary background also includes early research in electrochemical systems and biomimetics at CECRI. Dr. Carmel is a recipient of the CSIR-Senior Research Fellowship and has been recognized with a Best Paper Award at IEEE ICEDSS. Her academic interests span neuromorphic energy-efficient computing, device architectures, and the integration of 2D materials into nextgeneration electronics.

#### List of few Publications

- 1. Santhia Carmel et al, Journal of Applied Physics 2022, 131(14), 114301.
- 2. Santhia Carmel et al, Journal of Applied Physics, 2020, 127(9)
- 3. Santhia Carmel et al, Physica E: Low dimensional systems and Nanostructures, 2019, 114, 113630
- 4. Santhia Carmel et al, Physical Chemistry Chemical Physics, 2020, 252, 114454.



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Multi-Functional Nano-Materials Design ||
Materials and Composites || Bio- Medical
Devices || Sensors (SERS, SEIRA, SPR) ||
Cancer Theranostics || Flexible and
Wearable Materials

# **PUBLICATION STATISTICS**

(As of July-2025)

Total Number of Publications – 15 || Best Poster's – 2 || Conferences / School and Workshops – 17||Invited Lectures – 1||Citations – 54 || h-index – 4

# Dr. S. Asha, Ph. D.,

Dr. S. Asha is working as Assistant Professor in Department of Physics at Thiagarajar College of Engineering. She has a teaching experience of about six years as Assistant professor in various colleges and she is interested in both teaching and research. She did her postgraduation at Arul Anandar college, affiliated to Madurai Kamaraj University where she got graduated with first rank and distinction, as a part of post graduate project she worked on Non-Linear interactions on Photonic crystals, which received the Student Project Fellowship Tamil Nadu state council of Science and Technology. She completed her M. Phil degree at Madurai Kamaraj University. She completed her doctorate in Physics at Madurai Kamaraj University Women Scientist-A (WOS-A/PS-46/2012(G) program of Department of Science and Technology, India. As a part of her research she prepared various Bio Nano structures for sensing (SERS), cancer thermal therapy and bone tissue regeneration application. She did her Ph.D. work in collaboration with UGC-DAE, CSR, Indore and National Chemical Laboratory, Pune. Being an experimental Physicist she is experienced in preparing various nanomaterials and structures and has hands-on experience in various characterization techniques such as FTIR, Raman spectroscopy, AFM, XRD, SEM, TEM, MTT Assay. At present her areas of research interests lie in the preparation of novel functional materials for costeffective self-powered sensors, biosensors, theranostics and bone tissue regeneration applications. Dr. S. Asha is a highly enthusiastic person who was always fascinated in applying basic science towards biomedical applications and she is highly interested in taking both research and teaching in parallel.

#### List of few Publications

- 1.S. Asha A. Nimrodh Ananth, Sujin P. Jose and M. A. Jothi Rajan, Materials Science and Engineering B, 2020, 252, 114454.
- 2.S. Asha, A. Nimrodh Ananth, Sujin P. Jose et al, Applied Nanoscience, 2018, DOI: 10.1007/s13204-0180803-
- 3.S. Asha, A. Nimrodh Ananth, Sujin P. Jose and M. A. Jothi Rajan Biomedical Physics and Engineering Express, 2018,4, 065032.
- 4. S. Asha et al, International journal of nanotechnology, 2017,16: 1760034.
- 5. S. Asha et al, Adv. Nat. Sci.: Nanosci. Nanotechnol, 2017, 8: 035015.

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Magnetostriction || Fe-Ga alloys (Galfenol) || Arc melting || Microstructure analysis || Quenching effect || Actuator materials || Structural and magnetic properties|| Functional materials || Phase transitions || Smart sensors

#### **PUBLICATION STATISTICS**

(As of July-2025)

Total Number of Publications – 14 || Conferences / School and Workshops – 35|| Citations – 121 || h-index – 7 || i-10 -index – 6

# Dr. V. Vijayanarayanan, Ph. D.,

Dr. V. Vijayanarayanan is a dedicated academic and materials physicist with expertise in magnetic materials, sensor technologies, and smart materials. He began his academic journey at Govt. Arts College, Ooty, where he completed both his B.Sc. and M.Sc. in Physics. During this time, he worked on cosmic ray detection using plastic scintillators at the Cosmic Ray Laboratory, TIFR, Ooty, gaining early exposure to experimental techniques and high-precision instrumentation. He went on to complete an M.Phil. in Physics at V.H.N. Senthikumara Nadar College, Virudhunagar, focusing on the synthesis of CdO thin films using nebulizer-based spray pyrolysis and evaluating them for gas sensing. This research marked his transition into thin film and applied materials science.

Dr. Vijayanarayanan earned his Ph.D. in Physics at Thiagarajar College of Engineering (TCE), Madurai, with a focus on magnetostrictive materials, particularly Fe-Ga and rare-earth-doped alloys. His doctoral research was conducted in collaboration with the Defence Metallurgical Research Laboratory (DMRL), DRDO, Hyderabad, enabling advanced investigations into structural, magnetic, and thermal properties of these materials.

Currently, he serves as Assistant Professor at TCE, where his research covers magnetic sensors, spintronic materials, and thin film technologies. Actively involved in FDPs, workshops, and student mentoring, Dr. Vijayanarayanan combines experimental rigor with theoretical insight. His journey from TIFR to DRDO collaborations reflects his sustained commitment to scientific innovation in material physics.

#### **List of few Publications**

- 1. Vijayanarayanan V, Aravindan V, Karuppasamy B, Physica Scripta. 2024, 99 (8): 085979.
- 2. Aravindan V, Vijayanarayanan V, Karuppasamy B, Mahendran M, Mat. Tod. Com., 2024, 39:108599.
- 3. Vijayanarayanan V, Aravindan V, Mahendran M, Physica Scripta, 2022, 97(11):115807.
- 4. Vijayanarayanan V, Mahendran M, Ind. J. Pure & App. Phy., 2022, 60(8):627-33.
- 5. Aravindan V, Vijayanarayanan V, Mahendran M, Mat. Sci. Semicon. Proces., 2022, 150:106909.

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Thin Films and Coatings || Materials Synthesis and Composites Materials || Energy Harvesting and Storage Devices || Sensors || Instrumentation & Programming

#### **PUBLICATION STATISTICS**

(As of July-2025)

Total Number of Publications – 11  $\parallel$  FDPs – 4  $\parallel$  Conferences / School and Workshops – 32  $\parallel$  Citations – 37  $\parallel$  h-index – 3

# Dr. B. Karuppasamy, Ph.D.,

Dr. B. Karuppasamy is an Assistant Professor in the Department of Physics at Thiagarajar College of Engineering, Madurai. He completed his M.Sc. School of Physics at Madurai Kamaraj University and M.Phil., in VHNSN College, Virudhunagar. He earned his Ph.D. at Thiagarajar College of Engineering, focusing on electrical and optical studies of nanostructures for higherficiency solar cells.

As part of his research, he developed a custom automated nebulized spray pyrolysis system using Arduino and JAVA GUI to fabricate transparent conducting oxide thin films like FTO and ITO. He also synthesized antimony tin oxide (ATO) nanoparticles through various wet chemical methods. His work extended to dye-sensitized solar cells (DSSCs), examining Al-ion electrolytes and natural dye sensitizers to enhance device performance.

Dr. Karuppasamy is an experimental physicist with expertise in UV-Vis, UV-DRS, FTIR, and solar simulators for I–V measurements. He has built custom instruments such as spin coaters and measuring units using Arduino, Processing, and LabVIEW. He is proficient in C++, HTML, hardware, and networking. His research focuses on functional materials for energy harvesting and storage, thin films, coatings, and sensor development. He aims to create cost-effective and scalable renewable energy solutions. His work has been published in renowned journals including Solar Energy, Materials Research Express, Physica Scripta, and Journal of Solid-state Electrochemistry, highlighting his dedication to interdisciplinary innovation.

#### **List of few Publications**

- 1. Karuppasamy Bet al, Physica Scripta, 2024, DOI: 10.1088/1402-4896/ad623f.
- 2. Aravindan V, Vijayanarayanan V, Karuppasamy B, et al, Materials Today Communications, 2024, 39: 108599.
- 3. Karuppasamy B, Shenbagabalakrishnan B, Gayathri V, Solar Energy, 2022, 236: 608-612.
- 4. Karuppasamy, Balasubramanian K, Gayathri V, Materials Research Express, 2019, 6: 1250k6.
- 5. Karuppasamy et al, Journal of Solid State Electrochemistry, 2023, 27: 1001–1009.

*Q-AATRAL-2025* 



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Multi-Functional Materials ||
Microwave Devices || Ceramic
Materials || Optoelectronic Devices ||
Multiferroic Materials || Energy
Devices

# PUBLICATION STATISTICS

(As of July-2025)

Total Number of Publications – 20 || Conferences / School and Workshops – 25|| Citations – 357 || h-index – 10

# Dr. M. Dhilip, Ph. D, PDF.,

Dr. M. Dhilip is working as Research Faculty Assistant Professor in Department of Physics at Thiagarajar College of Engineering. He has a research experience of about eight years as Research Fellow in various institutes and he is interested in both research and teaching. He did his M.Sc Materials Science at College of Engineering (CEG) Campus, Anna University, as a part of post graduate project he worked superconducting materials. He completed his M. Tech Ceramic Technology at Alagappa College of Technology (ACTech) Campus, Anna University, which received the Student Post Graduate Fellowship from UGC, as a part of M.Tech project he worked Project Fellow in Saint Gobain Refractories, Palakkad, Kerala. He completed his doctorate in Physics at SRM Institute of Science and Technology (SRMIST) under project of DST-SERB, India. As a part of his research he prepared various multiferroic and Double perovskite materials for multifunctional application. He did his Ph.D. work in collaboration with IISC Bangalore, CSIR-CECRI, DRDO, Pondicherry University and IITM. Being an experimental Physicist he is experienced in preparing various materials and has hands-on experience in various characterization techniques such as XRD, Raman spectroscopy, UV-DRS, VSM, SEM-EDS, PL, XRF. At present his areas of research interests lie in the preparation of novel functional materials for costeffective Perovskites materials, Microwave devices, Sensors and energy storage applications. Dr. M. Dhilip is a highly enthusiastic person who was always fascinated in applying basic science towards Multifunctional applications and he is highly interested in taking both research and teaching in parallel.

#### **List of few Publications**

- 1. Dhilip M et al, Solid State Sciences, 2025, 107825.
- 2. Dhilip M et al, Ceramics, 2024, 2006-2023.
- 3. Dhilip M, Sundaramurthy R, Raji R K, Ramachandran T, et al, Materials Today Communications, 2024,108120.
- 4. Dhilip M et al, Journal of Materials Science: Materials in Electronics, 2023, 1462
- 5. Dhilip M, Punitha S, Rameshkumar R et al, Applied Physics A, 2022, 324.

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Nanostructured Materials and Composites | Electrospun materials Electrocatalytic CO<sub>2</sub>RR & HER | Energy Conversion and Storage Devices | Functional Oxides and Ferrite Composites

#### **PUBLICATION STATISTICS**

(As of July-2025)

Total Number of Publications – 20 || National/ International Presentations – 29 || Seminar, conference, FDP – 23 || National/ International Webinars – 81 || Book publications – 09 || Citations – 61 || h-index – 4

# Dr. Ashwin Sudhakaran, Ph. D., PDF.,

Dr. Ashwin Sudhakaran currently serves as an Assistant Professor in the Department of Physics at Thiagarajar College of Engineering, Madurai. With a solid academic and research foundation, he adopts a multidisciplinary approach to teaching, experimental research, academic mentoring. He earned his Ph.D. in Physics from Karpagam Academy of Higher Education, Coimbatore, where his research focused on the development of multiphase ferrite nanocomposites for applications in permanent magnets and photonics. He subsequently pursued a Postdoctoral Fellowship at the Centre for Nano and Material Sciences (CNMS), Jain (Deemed-to-be University), Bangalore, where he worked on the synthesis of bimetallic and electrospun ternary transition metal oxide nanofiber catalysts for CO, electroreduction and the hydrogen evolution reaction (HER).

Dr. Ashwin has extensive hands-on experience in a wide range of materials characterization techniques, including XRD, SPM (AFM & MFM modes), FTIR, SEM, and XPS. He is also proficient in electrochemical and thermal analysis techniques, such as CH Instruments (1760e), GC 1100, TGA, and STA. His research interests span multifunctional and nanostructured materials, electrospun materials for electrocatalytic CO, RR and HER, energy conversion and storage, and functional oxide and ferrite composites. He has made significant contributions to the academic community through journal and book publications, conference presentations, collaborative research projects, and by organizing various workshops and faculty development programs, reflecting his dedication to fostering interdisciplinary learning and scientific outreach.

#### **List of few Publications**

- 1. Sudhakaran A, Sudhakaran A, E Sivasenthil et al, Materials Chemistry and Physics, 2024,318: 129290
- 2. Sudhakaran A, Sudhakaran A, E Sivasenthil et al et al, Journal of Physics and Chemistry of Solids, 2023, 174: 111134
- 3. Sudhakaran et al, Journal of Materials science, 2025, 60, : 8205-8220
- 4. Sudhakaran et al, Journal of Materials Research, 2023,8: 1239-1253
- 5. Sudhakaran et al, Journal of Material Science: Materials in Electronics, 2023, 34: 104

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# EPICENTERS OF RESEARCH

# CENTRE OF EXCELLENCE IN MATERIALS RESEARCH AND ENERGY SOLUTIONS (Coemres)

Faculty Co-ordinators: Dr. M. Mahendran and Dr. S. Karthick prabhu

Faculty in-charge: Dr. P. Sivakumar

# **About the Centre**

**CoEMRES** – A Vibrant Research Centre at TCE, Madurai

The Centre of Excellence in Materials Research for Energy and Sustainability (CoEMRES) is a dynamic research hub established within the Department of Physics at Thiagarajar College of Engineering (TCE), Madurai. It builds upon the legacy of the Materials Science Research Laboratory, founded in 2008.

Led by a department-level coordinator and supported by two dedicated faculty members, CoEMRES focuses on pioneering research in advanced materials and emerging technologies aimed at addressing the global demand for clean and sustainable energy. Its core research areas include semiconductors, smart materials, nanomaterials, and multifunctional composites.

Beyond research, CoEMRES plays a pivotal role in nurturing the next generation of scientists and innovators in materials science and energy technologies. It offers hands-on training, internships, workshops, and project opportunities for graduate and doctoral students, fostering both academic excellence and industry readiness.



# **Objectives of CoEMRES:**

- To design and synthesize advanced nanostructured materials, smart materials, and composites for energy generation, energy storage, and environmental applications.
- To build sustainable materials capable of fulfilling multiple roles thereby enabling integrated, scalable, and eco-friendly solutions for future energy challenges.
- To foster collaborative research by connecting academia, industry, and research organisations, with an emphasis on green technologies and sustainable energy solutions.
- To enhance research capacity through FDPs, workshops, interdisciplinary training, hands-on experimentation, and eco-friendly prototype products

# **Origin of CoEMRES:**

**2008:** Inception as Materials Science Research Laboratories:

The research journey began in 2008 with the establishment of the Materials Science Research Laboratories under the Department of Physics, focusing on the synthesis and characterization of materials for diverse applications.

**2022–2023:** Launch of Energy Materials and Electrochemical Research:

Recognizing the rise of clean energy, the lab expanded into energy storage and conversion—exploring batteries, supercapacitors, fuel cells, and hydrogen production using advanced electrochemical workstations.

**2025:** Formalisation as the Centre of Excellence in Materials Research and Energy Solutions (CoEMRES):

The lab's transformation into a formal research centre in 2025 marked its expanded focus, enhanced infrastructure, and commitment to sustainable energy through advanced material development.



# **Scientific Impact**

CoEMRES has made notable strides in advanced materials and sustainable energy, publishing extensively in reputed journals. Its research—ranging from energy storage and hydrogen generation to thin films and multifunctional materials—tackles global scientific challenges. The Centre's steady output underscores its dedication to innovation and sustainability.

# Nuggets of recent findings

- 1. P Sundararajaperumal, M Mahendran, P Velusamy, Ikhyun Kim, Surfaces and Interfaces, 2025, 65, 106410.
- 2. P Sundararajaperumal, P Velusamy, M Mahendran, P Sivaprakash, Ceramics International, 2024, 50, 18, 34173-34183.
- 3. S Karthickprabhu, P Sundararajaperumal, M Mahendran, Dhanasekaran Vikraman, Sajjad Hussain, Khawla Ahmed Alhebsi, Ali Abdulkareem Alhammadi, Hyun-Seok Kim, K Karuppasamy, Akram Alfantazi, Journal of Power Sources, 2025, 648, 237378.
- 4. S Jayanthi, M Vahini, S Karthickprabhu, A Anusuya, N Karthik, K Karuppasamy, Tholkappiyan Ramachandran, A Nichelson, M Mahendran, B Sundaresan, Dhanasekaran Vikraman, Processes, 2024, 10 (12), 2174.
- M.Deepikaa, S. Karthickprabhu,
   K.Karuppasamy, M. Mahendran, Ionics, (2025).
   K.Aruna Devi, S. Karthickprabhu,
   K.Karuppasamy, M. Mahendran, Ionics, (2025).
- 7. Anusuya A.; Karthickprabhu S.; Mahendran M.; Vasanth Rajendiran Jothi; Palanivel Molaiyan; Aravindhan Selvaraj; Hyun-Seok Kim; Min Jae Ko; Karuppasamy K; Akram Alfantazi, Advances in Colloid and Interface Science, (2025).
- 8. Venkadeshkumar Ramar; Sivakumar Periyasamy; Prabhu Sengodan; Huijun Tan; Hao Zhang; Xianglong Zhang; Yasin Orooji, Coordination Chemistry Reviews (2025).
- 9. Sundararajaperumal; P Sivakumar; Pretika PA, M. Mahendran, Journal of Materials Science: Materials in Electronics (2025).
- 10. P. Sundararajaperumal; P Sivakumar; M. Mahendran, Venkadeshkumar Ramar, Journal of Hydrogen Energy (2025).
- 11. Pretika PA; P Sivakumar, M. Mahendran; Fouran Singh, Journal of Electroanalytical Chemistry (2025).

# CRYSTAL GROWTH RESEARCH LABORATORY (CGRL)

Faculty Co-Ordinator: Dr. M. M. TamilElakkiya

# **About the Laboratory:**

CGRL - A Thriving Research Laboratory at Physics Department, TCE, Madurai

The Crystal Growth Research Laboratory (CGRL) at Thiagarajar College of Engineering (TCE), Madurai, is a leading centre for cuttingedge research in crystal science, with a specialized focus on nonlinear optical (NLO) materials, shock wave-induced crystal growth, and crystals for photonic and biological applications. Building its strong foundation in materials research, CGRL explores novel crystal growth techniques to develop high-performance materials essential for next-generation optical and photonic technologies. The lab provides a collaborative environment for research scholars and students, offering opportunities for handsexperimentation, advanced material on characterization, and interdisciplinary projects in the rapidly evolving field of photonic materials.

**Scientific Impact** 

The Crystal Growth Research Laboratory (CGRL) has made significant contributions in the field of crystal science, with impactful research spanning nonlinear optical materials, shock wave-induced crystals, photonic and biological applications.

The laboratory's work, published in reputed national and international journals, addresses key challenges in optics, photonics, and material engineering.



Through innovations in crystal growth techniques and material synthesis, CGRL continues to support the development of next-generation technologies for optical communication, laser systems, and sensor applications, reflecting its commitment to scientific excellence and technological advancement.

# **Objectives of CGRL:**

- To design and grow high-quality single crystals, including nonlinear optical and photonic materials, through advanced crystal growth techniques tailored for next-generation optical technologies.
- To explore and develop novel materials via shock wave-assisted synthesis methods, enabling unique structural and functional properties for cutting-edge scientific and industrial applications.
- To advance research in crystal engineering for photonic and optoelectronic applications by integrating theoretical modelling, experimental synthesis, and precision characterization.
- To promote interdisciplinary collaboration between physicists, chemists, material scientists, and engineers to address challenges in crystal growth and photonic device integration.
- To strengthen research capacity and innovation through specialized training programs, workshops, student research projects, and hands-on experience in crystal growth and material characterization.

 To contribute to sustainable technology development by creating crystals and materials that enhances the efficiency, durability, and eco-compatibility of photonic and optical systems.



# Nuggets of recent findings:

- 1. Manoj. K.S and M. Tamilelakkiya, 2,4,6 Triaminopyrimidinium salicylate, CSD Communication, doi: 10.5517/ccdc.csd.cc2p4x81(2025)
- 2. Manoj. K.S, A. Mythili, Selva Ganapathy M, M. Tamilelakkiya, Synthesis, crystal growth, and physicochemical characterization of hydrogen bond rich multi-component hydrous salt co-crystal tetrakis (2,4,6-triaminopyrimidinium) tetrakis (4-nitrophenolate) 4-nitrophenol pentahydrate (ANNH) for NLO applications, J Mater Sci: Mater Electron (2025).
- 3. Manoj. K.S and M. Tamilelakkiya, tetrakis (2,4,6-triaminopyrimidinium) tetrakis (4-nitrophenolate) 4-nitrophenolpentahydrate, CSD Communication, doi: 10.5517/ccdc.csd.cc2ndnk9 (2025).
- 4. P. Justin, M. Tamilelakkiya, A. Mythili, P. Velusamy, and K. Anitha, Investigation on the structure, optical, thermal, Z-scan, and DFT characteristics of nitrobenzimidazolium phthalate monohydrate single crystal, J Mater Sci: Mater Electron (2025) 36:770.

# SMART MATERIALS RESEARCH LABORATORY

Lab Established by: Prof. M. Mahendran Faculty in-charge: Dr. V. Aravindan

#### **About the Centre**

Smart Lab – Located within the Department of Physics, this lab focuses on research involving smart and nanoscale materials for sensors, actuators, and energy—absorption applications Legacy & Impact

Prof. M. Mahendran effectively founded and nurtured the Smart Materials Lab at TCE through:

- · Leading significant interdisciplinary research projects across various funding agencies including, DRDO, CSIR, ISRO, DST, and UGC.
- · Establishing the research infrastructure and facility ecosystems (synthesis setups, characterization tools, computational modelling) that enabled advanced smart materials research.
- Building academic capability by mentoring a generation of researchers in smart materials-based studies and applications.

#### **Research Infrastructure:**

Measurement and synthesis instruments: Vacuum arc melting unit, furnaces (tubular and box-type), electromagnets, acoustic-attenuation setup, ball milling and rolling machines, scanning tunneling and optical microscopes, DSO (digital storage oscilloscope).



Software tools: VASP, WIEN2k, NI-LabVIEW (with DAQ interface), Materials Studio, MATLAB, MathCAD, Ansys, and Gaussian-03W for virtual instrumentation and computational modelling.

Research Focus & Projects

#### **Completed Work:**

- Energy-absorption studies of smart materials
- Magneto-Rheological Fluids (MRF) for mechanical dampers
- Ferromagnetic Shape Memory Alloys (FSMA) Ni-Mn-Ga & Magnetostrictive Fe-Ga alloys for sensors and actuators
- Fabrication and characterization of smart composites and nanoscale materials

- Exploring field-induced correlation effects in quantum dots (SQDs)
- Carbon NanoTubes (CNTs) for hydrogen storage systems
- Half-metallic Heusler alloys for spin-based devices

# **Ongoing Research:**

- Quantum computing for health care applications
- Theoretical framework on perovskites for hydrogen storage, photovoltaics, spintronics, and thermoelectrics

# **Key Research Contributions:**

Dr. Mahendran led several high-impact funded research projects that built the lab's research identity:

No.	Title	Sponsoring Agency	Amount (₹
			Lakhs)
1	Ferromagnetic Shape Memory Alloys	UGC-DAE CSR,	13.00
		Indore	
2	FSMA Polymer Composites	DST – Women	26.00
		Scientist Scheme	
3	Ferromagnetic Shape Memory Alloy Thin	SERB-DST, New	39.00
	Film	Delhi	
4	Magnetic & Structural Properties of Co- and	UGC-DAE CSR,	13.50
	Fe-Substituted Smart Materials	Mumbai	
5	Characterization of Ni-Mn-Ga Single	UGC-DAE CSR,	07.00
	Crystals	Indore	
6	Acoustic-Assisted Magnetic Field-Induced	CSIR, New Delhi	14.00
	Actuation in Ni-Mn-Ga		
7	Electronic Properties of Quantum Dot	DST, New Delhi	09.00
	Structures		
8	Design of Magnetic Shape Memory Alloy	UGC, New Delhi	09.00
	Actuator		
9	Nanostructured Ferromagnetic Shape	DRDO, New Delhi	09.00
	Memory Alloys		
10	Acoustic Attenuation in FSMA Composites	DRDO, New Delhi	15.00
11	Characterization, Optimization, and	ISRO, Bangalore	13.00
	Fabrication of FSMA Composites		



# Nuggets of recent findings

- 1. M.N. Kumar, V. Aravindan, N. Laihnuna, M. Mahendran, "Rare earth-based LaCoCrZ (Z=In, Sn, Sb) equiatomic quaternary Heusler alloys: Materials for high-temperature thermoelectrics," Journal of Rare Earths.
- 2. P. Sundararajaperumal, M. Mahendran, P. Velusamy, I. Kim, "Incorporation of W<sup>6+</sup> metal ion in CoAl<sub>2</sub>O<sub>4</sub> for enhanced green hydrogen production: A synergetic effect and phase contributions," Surfaces and Interfaces, 65, 106410.
- 3. S.R. Sagitha, V. Aravindan, J.S. Rani, M. Mahendran, "Green synthesis and characterization of nano selenium using the extract of Phyllanthus emblica," Measurement: Energy, 100051.
- 4. S.R. Sagitha, V. Aravindan, M. Mahendran, M.N. Kumar, "Numerical simulations of the efficiency of BiFeO<sub>3</sub> perovskite solar cells," Applied Physics A, 131 (4), 333.
- 5. P. Sundararajaperumal, P. Velusamy, M. Mahendran, P. Sivaprakash, "Influence of Nd<sup>3+</sup> ions modified CoAl<sub>2</sub>O<sub>4</sub> nanomaterials for high-efficiency dye degradation application," Ceramics International, 50(18), 34173–34183.
- 6. V. Aravindan, V. Vijayanarayanan, B. Karuppasamy, K. Sakthipandi, M. Mahendran, "First-principles study on rare earth-based equiatomic quaternary Heusler alloys YbCoCrSb and YbCoTiSn: New candidates for spintronics," Materials Today Communications, 39, 108599.
- 7. K. Raji, T. Ramachandran, M. Dhilip, V. Aravindan, J.S. Punitha, F. Hamed, M. Mahendran, "Integrating experimental and computational insights: A dual approach to Ba<sub>2</sub>CoWO<sub>6</sub> double perovskites," Ceramics, 7(4), 2006–2023.
- 8. M.S. Mousa, H.Al Dmour, E.K. Jaradat, O.Y. Al-Madanat, A. M.D., B. Zaidi, V. Aravindan, M. Mahendran, "Studying the effect of transport layers on ZrS<sub>2</sub>/MEH-PPV solar cells: Using SCAPS-1D software," East European Journal of Physics, 419–426.

# Research Infrastructure

• Make/model: HHV

• Vacuum Level: High vacuum (10<sup>-6</sup> mbar).

• Substrate Sizes: Up to 6 inches in diameter

• Temperature Control: Substrate heating up to 500°C

• Cooling: Water – cooled chamber and components

RF sputtering is a versatile technique widely used for the thin film deposition of semiconductors, metals, and metal oxides. It enables the formation of high-purity, uniform coatings essential for applications in electronics, optics, and various high-performance devices. Through consultancy services, industries and research institutions can benefit from expert guidance in process optimization—tailoring sputtering parameters to meet specific application requirements, thereby improving quality, uniformity, and deposition efficiency. Additionally, consultancy support extends to material development, assisting in the design and fabrication of novel coatings and composite films for demanding applications in fields such as aerospace, automotive, and biomedical engineering, where materials must meet stringent functional and environmental performance standards.

# 1. RF/DC Magnetron Sputtering System



# 2. Thermal Evaporation Unit



Make/model: HHV

• Vacuum Level: High vacuum (10<sup>-6</sup> mbar).

• Operating Temperature: Over 3500°C.

The Thermal Evaporation Unit is a fundamental tool for thin film deposition, widely used in the fabrication of metal, semiconductor, and dielectric coatings. This technique enables precise control over film thickness and composition, making it ideal for applications in microelectronics, optics, and material science. Consultancy services can play a critical role in optimizing film properties by refining deposition parameters to enhance film quality, deposition rate, and process reproducibility key factors for industries that demand high-quality coatings at scale. Additionally, expert consultation can support the development of custom materials and specialized films tailored for advanced applications, including next-generation energy storage devices, highly sensitive sensors, and complex photonic structures, ensuring that the thermal evaporation process is both efficient and application-specific.

# • Operating Temperature: Over 3500°C

• Chamber: 304 Stainless Steel, copper base and copper water-cooled crucible.

• Electrode: Tungsten rod.

• Power: 208-240 V. 50 Hz, 40 kW.

The Arc Melting Furnace is essential for alloy and material synthesis, particularly in high-temperature and high-energy material studies. It is widely used for the fabrication of advanced alloys required in demanding applications such as high-performance tools, heat exchangers, and corrosion-resistant components. Consultancy services can assist industries in developing custom alloy compositions and optimizing melting and solidification processes to reduce defects and enhance material quality. Expert guidance ensures that the final products meet specific mechanical, thermal, or electrical property requirements, making the process more efficient and application-driven.

# 3. Arc Melting unit



# 4. Electrochemical Workstation (Micro Auto lab with FRA2)



• Make: Metrohm AutoLab Electrochemical Workstation (PGSTAT204).

• Potential Range: ±10 V

• Current Ranges: 10 nA to 100 mA.

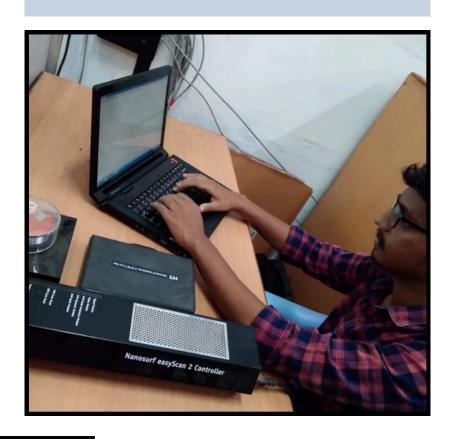
Input Impedance: >10<sup>12</sup> Ω
 Bandwidth: 10 mHz to 1 MHz

The Electrochemical Workstation is a vital tool for conducting fundamental electrochemical studies, supporting advanced research in batteries, fuel cells, supercapacitors, and sensors. It enables precise performance testing and optimization of energy storage devices, which is critical for applications ranging from portable electronics to large-scale energy systems. Consultancy services can provide expertise in improving device efficiency, especially in fuel cell applications for the automotive and aerospace sectors, as well as in selecting and evaluating materials for high-performance supercapacitors. This guidance ensures enhanced reliability, functionality, and innovation in electrochemical technologies.

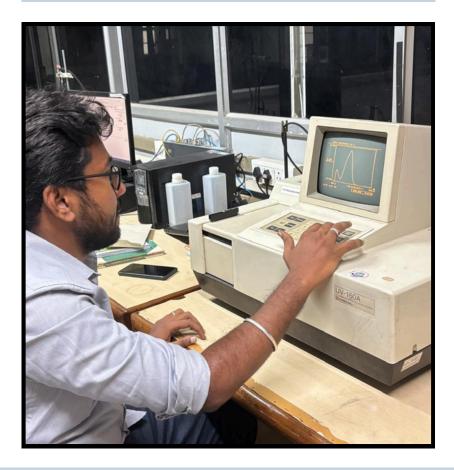
- Make: Nanosurf easyScan.
- Scanning Area: Typically, 100 nm x 100 nm at atomic resolution.
- Sample types: Conductive materials

The Scanning Tunneling Microscope (STM) is a powerful instrument for atomic and molecular imaging, allowing detailed analysis of surface topography electronic structure at the nanoscale. It plays a crucial role in the study of 2D materials, nanostructures, and thin films. Consultancy assist advanced services can in nanofabrication techniques using STM, as well as in developing effective surface protection strategies for sensitive materials. Expert guidance enhances the precision and of surface research, scope enabling innovation in fields such as nanoelectronics. catalysis, and materials science.

# **5. Scanning Tunnelling Microscope**



# 6. UV-Vis Spectroscopy



- Model: UV -160A
- Spectral Band width: 2nm
- Wavelength readability: 0.1nm increment

The UV-Visible Spectrometer is a key analytical tool used for chemical and biochemical analysis, as well as for studying the optical properties of nanomaterials such as quantum dots, nanoparticles, and thin films. It is widely employed in determining the band gap of semiconductors and evaluating the photocatalytic activity of nanomaterials. Consultancy services can support advanced research and industrial applications by offering expertise in spectral data interpretation, material characterization, and purity testing particularly in pharmaceutical, chemical, industries—ensuring high standards of quality and performance.

• Model: TG/DTA6300

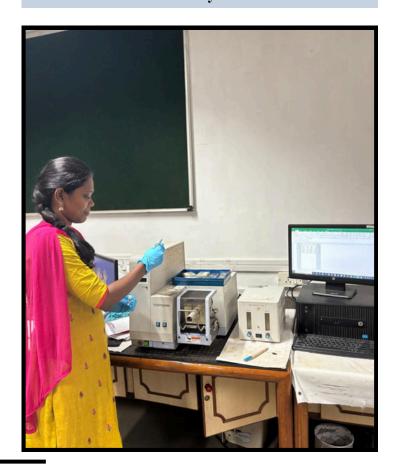
• Sample loading weight: 200mg

(Maximum)

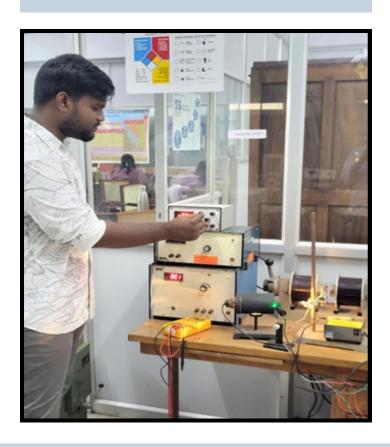
• Temperature Range:1500°C

TG/DTA (Thermogravimetric Analysis/Differential Thermal Analysis) is a powerful technique for studying thermal stability, decomposition behavior, and phase transitions in a wide range of materials. including polymers and composites. It provides critical insights into melting behavior and thermal responses under controlled conditions. Consultancy services can assist industries in monitoring thermal stability for quality control, particularly in the polymer, pharmaceutical, and food sectors. Additionally, expert guidance is valuable in selecting materials for high-temperature applications, ensuring both performance and reliability in demanding environments.

# 7. Thermogravimetry Differential Thermal Analysis



# 8. Hall effect setup



Make: Self-assembled.
Power Supply: 0 – 100V.
Electromagnet: 7.5 G.
Gauss meter: 0-20 k.

The Hall Setup is an essential tool for analyzing the electrical and magnetic properties of materials, including the characterization of n-type and p-type semiconductor behavior. It. enables precise measurements of magnetic susceptibility, carrier concentration, and magnetoresistance, which are crucial for developing advanced electronic and magnetic materials. Consultancy services can provide specialized support in interpreting these properties for novel materials and offer guidance on Hall-effectbased magnetic sensing technologies, particularly valuable for applications in the automotive and aerospace industries where precision and reliability are critical.

• Maximum pressure: 20 Tone.

Operation: Manual.Diameter: 10 to 20mm.

• Width x Height x Diameter: 380x650x300 mm.

The Pelletisation Setup Apparatus is crucial for optimizing drug pellet formulation, enabling controlled drug release through precise control of pellet porosity, density, and mechanical strength. It is widely used in pharmaceutical and industries to enhance chemical product consistency and performance. Consultancy services can assist in improving pelletization efficiency, ensuring better process control and product quality. Additionally, the setup is valuable in battery manufacturing, where expert guidance can support the optimization of electrode material pelletization processes, leading to improved energy storage performance and manufacturing efficiency.

# 9. Palletisation setup Apparatus



Make: Self assembled.Aero let size: 0.5 mm.Heating: Resistive heating.

• Control: Manual.

A self-made spray coating setup offers flexible and cost-effective capabilities for research in thin film deposition, surface modification, and material coating. It enables precise control over film thickness, uniformity, and surface coverage, making it suitable for applications in sensors, photovoltaics, biomedical devices, and Research superhydrophobic surfaces. applications include the deposition polymers, nanoparticles, and functional coatings on various substrates. Consultancy services can support the optimization of spray parameters such as nozzle design, spray distance, pressure, and solution properties to improve coating quality and reproducibilty. Additionally, expert guidance can assist in adapting the setup for specific material systems scaling the process for industrial applications.

# 10. Spray coating setup



• Model: Technico-Tubular Furnace.

• Maximum Temp.: 1700 °C.

• Display Type: Analog.

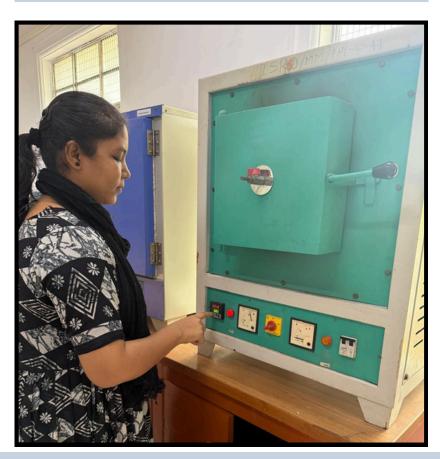
• Furnace medium: N<sub>2</sub>/Ar.

The vacuum furnace is a high-precision thermal processing instrument used for heat treatment, sintering, annealing, and brazing of materials low-pressure under controlled or vacuum environments. Its research capabilities include studying high-temperature phase transformations, developing advanced alloys, synthesizing ceramic materials, and processing materials sensitive to oxidation or contamination. In consultancy, experts can assist in optimizing temperature profiles, vacuum levels, and gas atmospheres to achieve desired material properties such as purity, density, and mechanical strength. Industries such aerospace, electronics, metallurgy, as advanced manufacturing benefit from guidance on process optimization, material selection, and scale-up strategies for high-performance and contamination-free thermal treatments.

# 11. Vacuum furnace



# 12. Muffle furnace



• Model: Technico.

• Maximum Temp.: 1200 °C.

• Display Type: Digital.

• Furnace medium: Air.

The muffle furnace is a key instrument for high-temperature treatment ceramics, metals, and polymers, widely used in both research and industrial applications. It enables processes such as annealing, tempering, and stress relieving of metallic and composite materials under controlled heating conditions. Additionally, it supports the investigation of crystal structure changes and phase transitions in heat-treated materials, making it essential for material development, thermal stability studies, and quality control.

• Model: PM 100.

• Grinding Jar Volume: 12 ml to 500 ml.

• Speed: 100-650/min.

• G. Force: 33.3g.

The Ball Milling Unit is a versatile tool used for particle size reduction, nanomaterial synthesis, and the refinement of materials at the micro and nanoscale. It enables the study of size-dependent material properties, which are critical in fields like electronics, catalysis, and energy storage. In research, it supports the development of advanced materials with tailored structural and functional characteristics. Consultancy services can provide guidance on optimizing milling parameters, selecting appropriate milling media, and scaling up processes for industrial-scale production. Additionally, expert support is available for ball milling applications in solidstate battery processing, ensuring efficient material blending and enhanced electrochemical performance.

# 14. Coin cell (battery) preparation unit



# 13. Ball Milling Unit



- Crimping die: Coin cell, CR 2032, CR2025, CR2016.
- Pressure: Max. 8 metric ton hydraulic pressure.
- Dimension: 232 mm x 190 mm.
- Weight: 30 kg.

The Coin Cell Preparation Unit is essential for the fabrication and testing of anode and cathode materials used in Li-ion. Na-ion, and emerging next-generation batteries. It supports detailed studies on electrode composition, the influence of binders, and the role of conductive additives in improving battery performance. The unit also facilitates the optimization of coating techniques to ensure uniform electrode thickness high and reproducibility. Consultancy services can assist researchers and industries in refining coin cell fabrication techniques for both R&D and mass production, offering process optimization strategies for consistent electrode preparation, assembly, and electrochemical testing to achieve reliable and scalable battery performance

• Make: Universal Vacuum chuck.

• Speed Range: 100 -10,000 rpm.

• Speed accuracy: ±1%.

• Acceleration: upto 80,000 rpm.

• Housing material: Corrosion free powder coated metal.

The Spin Coating Setup is a critical tool for fabricating uniform thin films used in optical, electronic, and biomedical applications. It enables precise control over film thickness and uniformity by adjusting parameters such as spin speed, coating time, and solution viscosity. This setup is also valuable for investigating multilayer coatings in advanced applications like sensors, displays, and photonic devices. Consultancy services offer expertise in high-precision coating techniques tailored for electronics and optics, along with optimization strategies to achieve process consistent, defect-free films that meet demanding performance and quality standards.

# 15. Spin coating setup



# 16. Glove box



Make: MBRAUNProcessing gas:Ar

• Gas purification Max: (1ppm H<sub>2</sub>O/O<sub>2</sub>)

• Integral leak Rate: (0.05vol%h)

• Per Ambient Temperature: 15°C-30°C

Glowbox offers robust research and consultancy capabilities, specializing in advanced materials, thin-film fabrication, and engineering. With expertise surface techniques like RF sputtering, spin coating, and nanomaterial synthesis, Glowbox provides tailored solutions for academic, industrial, and biomedical applications. The consultancy supports process optimization, equipment setup, and material characterization, enabling clients to achieve high-precision, applicationspecific outcomes.

• Model: Technico.

• Maximum Temperature: 200 °C.

Display Type: Digital.Furnace medium: Air.

The Hot Air Oven is a fundamental laboratory instrument used for thermal processing tasks such as drying, sterilization, and heat treatment of samples. In research, it plays a key role in studying thermal stability, moisture content, and the drying behavior of materials like polymers, pharmaceuticals, food products, and nanomaterials. Consultancy capabilities include optimizing drying protocols to enhance efficiency and product quality, advising on material compatibility with high-temperature environments. ensuring uniform and distribution for reliable results. Industries can also benefit from expert guidance in using hot air ovens for quality control, sterilization standards, and process validation in sectors such as pharmaceuticals, food, textiles, and electronics.

# 17. Hot Air Oven



# 18. Available Software Packages



b-initio Sackage imulation

- Wein2K
- Gaussian
- VASP
- Material Design & Discovery: Predicting new materials with desirable properties.
- Process Optimization: Simulating reaction mechanisms and optimizing synthesis routes.
- Failure Analysis: Understanding material degradation, corrosion, and mechanical failure.
- Energy Applications: Designing catalysts for fuel cells, solar cells, and batteries.
- Electronics & Optoelectronics: Band structure tuning for semiconductors, LEDs, and sensors.
- Pharmaceuticals & Chemicals: Drug interactions, molecular stability, and reaction kinetics.







Dr. V. Aravindan **Assistant Professor** 

Specialization: Theoretical Physics



**Professor and Head** Specialization: Quantum Computing



Mr. V. Veeraganesh **Assistant Professor Specialization: Quantum Mechanics** 



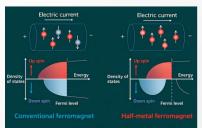
Dr. V. Vijayanarayanan **Assistant Professor** Specialization: Experimental Physics

**About Us** 

The Quantum Technology Group is dedicated to the design and discovery of novel quantum materials and devices through advanced theoretical and computational methods, including Density Functional Theory (DFT) and quantum many-body simulations. Our research spans magnetism, spintronics, quantum coherence, and their applications in computing, communication, sensing, and healthcare technologies. By aligning with the United Nations Sustainable Development Goals (SDGs), we aim to contribute to good health and well-being (SDG 3), industry innovation (SDG 9), and affordable and clean energy (SDG 7) through quantum-enabled solutions.

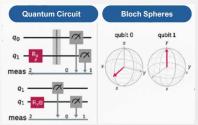
Research

#### Correlated Electron and Structural Effects on Spin Polarization in Half-Metals



We investigate and design half-metallic ferromagnets with 100% spin polarization at the Fermi level for advanced spintronic applications. Our research combines first-principles density functional theory (DFT) with many-body approaches to predict and tune their electronic, magnetic, and transport properties. Particular emphasis is placed on understanding spin-dependent band structures, exchange interactions, and the effect of chemical substitution and strain engineering on spin polarization. Furthermore, we develop computational models to explore spin injection efficiency, magnetoresistance effects, and stability under device-operating conditions. The goal is to establish robust design principles for materials that can serve as high-performance spin filters, magnetic tunnel junction electrodes, and building blocks for quantum spintronic devices.

#### Image Analysis using Variational Quantum Eigensolver Algorithm and IBM's Qiskit



Quantum computing, based on quantum mechanics, has the potential to revolutionize the medical field by assessing active cancer cells in a restricted area. The Variational Quantum Eigensolver (VQE) technique uses a quantum circuit with qubits, Pauli's gates, CNOT gates, Hadamard gates, image processing methods, Bloch sphere representation, and Schrodinger's time evolution equation to calculate Hamiltonian energy. Data from imaging of cancer cells can be encoded using a quantum circuit. The study used IBM Qiskit to simulate and build quantum circuits, extracting cancer image pixel intensity using quantum amplitude encoding. The study highlights the gap between theoretical quantum techniques and real healthcare applications, potentially leading to early diagnosis and treatment.

Ms. Thirisha C - Quantum Computing

Ms. S. Reema Sagitha - First-principles Study

Mr. Nandha Kumar M - Abinitio Calculations Mr. R.K. Jithesh - Density Functional Theory

**Contact Us** Q-AATRAL-2025

**Research Scholars** 



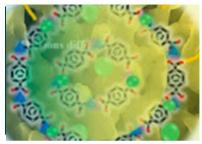




The Special Interest Group (SIG) on Energy Storage Materials at Thiagarajar College of Engineering is dedicated to advancing research in sustainable, high-performance energy storage technologies. We focus on designing, synthesising, and characterising novel electrode and electrolyte materials for batteries, supercapacitors, and hybrid devices. By combining experimental techniques with simulation tools, we aim to create efficient, eco-friendly, and scalable materials that support clean energy solutions. The SIG promotes interdisciplinary collaboration among students, researchers, and industry partners to foster innovation and help achieve national energy objectives. Its initiatives align with the United Nations Sustainable Development Goals (SDGs), especially in promoting affordable and clean energy (SDG 7) and encouraging industry, innovation, and infrastructure (SDG 9).

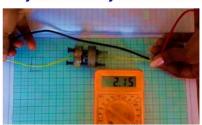
Research

#### Coral-Reef Ni-MOFs: Power from the Deep for Next-Gen Supercapacitors



Metal-Organic Frameworks (MOF's), due to their porous structures, tunability, crystal control, and chemical compositions, are useful in energy storage. Their organic framework boosts double-layer capacitance, while mixed inorganic frameworks add pseudocapacitance, creating a synergistic effect. This work used a simple wet chemical process to make Ni-doped Co/Fe-MOF@Fe<sub>2</sub>O<sub>3</sub>, showing improved electrochemical properties through Ni<sup>2+</sup> and Co/Fe-MOF synergy. Its coral-reef morphology and texture provide many active sites and facilitate electron and electrolyte movement. It achieved an excellent capacitance of 136.4 F g-1, energy density of 37.1 Wh kg-1, and power density of 700 W kg-1 at 1 A g-1, with 86.6 % retention after 5000 cycles. These results suggest its potential as an electrode in hybrid supercapacitors

#### Polymer Electrolytes for Enhanced Energy Storage Solutions



In lithium-polymer batteries, the electrolyte is a crucial component affecting ion transport, performance, stability, and efficiency. This study develops nanostructured composite polymer electrolytes (NCPEs) via solvent casting, using poly(vinyl chloride) (PVC), lithium bromide (LiBr), and silica (SiO2). Nano-Sio2 significantly increased ionic conductivity, reaching 10<sup>-5</sup> S/cm at 7.5 wt%, due to increased amorphicity from interactions with polymer, salt, and filler. X-ray diffraction showed both crystalline and amorphous phases, confirming improved ionic transport. The NCPEs also exhibited excellent thermal stability up to 334°C suitable for lithium-polymer batteries. A lithium-ion-conducting cell (Zn + ZnSO<sub>4</sub>.7H<sub>2</sub>O|PVC: LiBr: SiO<sub>2</sub>|PbO<sub>2</sub> + V<sub>2</sub>O<sub>5</sub>) with an open circuit voltage of 2.15 V demonstrated promising discharge performance. These electrolytes, with superior morphological and electrical properties, offer a pathway for advancing lithium-polymer battery technology.

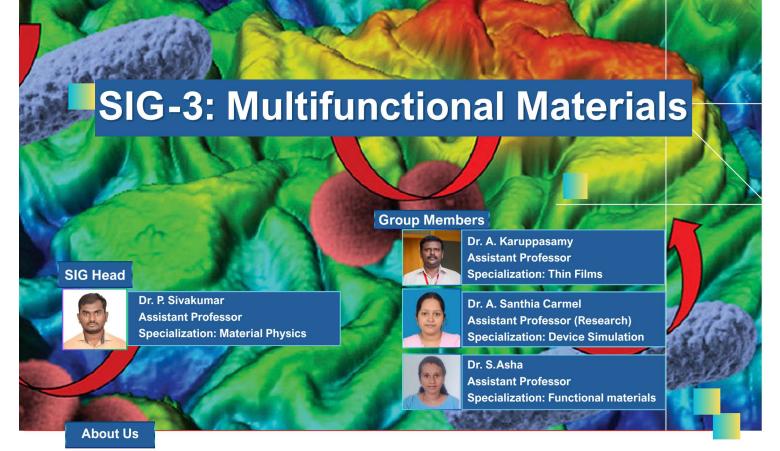
Mrs. A. Anusuya - Supercapacitors

Ms. M. Deepikaa - Water Splitting

Ms. K. Aruna Devi - Supercapacitors

Mr. B. Prabhu - Water Splitting

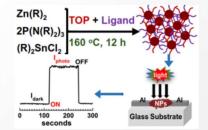




Our research group is advancing multifunctional materials in direct alignment with the United Nations Sustainable Development Goals (SDGs 3, 7, 9, 12). We design novel materials for efficient energy harvesting and storage, addressing affordable and clean energy (SDG 7). Our work in thin film technology enables precise nanoscale fabrication for next-generation electronics and sensor platforms, driving industry innovation (SDG 9). Using advanced semiconductor device simulations, we optimize multifunctional device architectures for performance and sustainability, supporting responsible consumption and production (SDG 12). We also develop smart biomedical materials for biosensors and implants to improve health outcomes (SDG 3). By combining theory, simulation, and experimental validation, our team accelerates the translation of scientific discovery into real-world solutions. Our research fosters technological progress in clean energy, sustainable industry, and healthcare. We are committed to scientific excellence and impactful innovation in support of the SDGs.

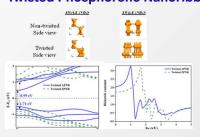
#### Research

# **Functional Materials for Energy Harvesting and Storage**



Our research group has developed a versatile chemical synthesis route for ternary semiconductor nanoparticles using commercially available precursors at relatively low temperatures. This method enables the production of highly stable, sub-10 nm particles with controlled stoichiometry and chalcopyrite structure, which can be deposited as uniform, few-monolayer-thick films. Subsequent modification with ion beams, spanning energies from keV to MeV, was employed to systematically tailor the structural, optical, and photoresponse properties of the thin films. By carefully selecting ion species and energies, we induced controlled defect formation, structural disorder, and recrystallization effects, resulting in tunable band gaps and enhanced broadband photo-responsivity, especially in the visible range. The observed changes in performance were closely correlated with the electronic energy loss mechanisms in the films. This approach demonstrates the potential of combining low-temperature chemical synthesis with ion beam engineering to optimize material properties for next-generation optoelectronic devices such as photodetectors and solar cells.

#### Twisted Phosphorene Nanoribbons-Tunable: Electronic and Optical Properties



**Research Scholars** 

Our research sheds light on the electronic and optical properties of twisted phosphorene nanoribbons (PNRs) for nanoscale device applications, using Density Functional Theory (DFT) simulations. We observed that the electronic bandgap of armchair phosphorene nanoribbons (APNRs) can be effectively scaled down through twisting, with a reduction of approximately 132 MeV per degree of twist. Additionally, the spectral response of twisted APNRs extends from the infrared (IR) region into the visible range, particularly in the armchair configuration. This twist-induced modulation results in a tunable optical bandgap and a significant increase in dielectric constant, enhancing their suitability for optoelectronic applications. These findings suggest that twisted APNRs are promising candidates for next-generation nanoscale optoelectronic devices, offering both structural flexibility and functional tunability.

Mr. P. Sundararajaperumal – Dye Degradation Ms. Pa. Prethika – Green Hydrogen Production

Mr. R. Bhuvanesh Kumar - Energy Applications Ms. P. Nivetha - Industrial Waste Water Management

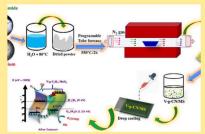
**Contact Us** 



Regenerative biomaterials and nanomaterials have emerged as transformative technologies in the fields of energy and biomedical applications, offering innovative solutions that align with the principles of sustainability and environmental stewardship. In the biomedical domain, regenerative biomaterials such as bioactive scaffolds, hydrogels, and biodegradable polymers are engineered to restore, replace, or regenerate damaged tissues and organs, accelerating healing processes and minimizing long-term complications (SDG3). Furthermore, in biomedical applications, nanomaterials are instrumental in targeted drug delivery, imaging, diagnostics, and antimicrobial treatments (SDG9). The integration of regenerative biomaterials and nanotechnology paves the way for sustainable and high-performance solutions that address critical global challenges in health care and clean energy (SDG13).

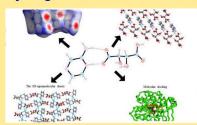
#### Research

#### **Green Energy and Environmental Applications**



Photoelectrochemical (PEC) systems are likely inefficient due to factors like charge carrier mobility, recombination rate, and solar light absorption. Fabricating semiconductor-metal sulfide nanocomposites and nanostructured materials can enhance solar radiation absorption, electron-hole separation, transport, and the generation of hydrogen (H2) and oxygen to address the world's energy challenge. The vanadium-doped (V) layered graphitic carbon nitride (g-CN)/MoS2 (MS) nanocomposite was synthesized using a two-step process of solvent evaporation and thermal condensation. This multilayer V-doped g-CN/MS nanocomposite degraded methyl red dye within 60 minutes under sunlight. Thanks to visible light absorption, the V-doped g-CN-MS nanostructure degraded the dye by 97.84%. We found that coating TiO2 nanorods with 3.0 wt.% V-doped g-CN/MS yielded a catalyst nanocomposite with a high photocurrent density of 23.72 mA/cm² and an H2 production rate of 4477 mol/h/cm². Additionally, the microstructure, optical absorption behavior, and electrical conductivity all contributed to these impressive PEC characteristics. The V-modified g-CN/MS nanocomposite structures are effective, well-regulated PEC catalysts, and this study offers insights into improving PEC water splitting and dye degradation.

### Hydrogen Bonds at Work: Building Blocks of a Novel Tartrate Crystal



The equimolar molecular adducts 2-aminopyrazinium hydrogen tartrate (APZHT) has been synthesized and inspected by the experimental and theoretical access. The molecular structure of APZHT was elucidated by single crystal X-ray diffraction analysis and it confirms the monoclinic crystal system with P21/n space group. To validate the observed experimental results and investigate the molecular properties of APZHT molecule, density functional theory (DFT) calculations have been carried out by Gaussian 09 program. Molecular structure optimization, vibrational frequency calculation and molecular properties such as Mulliken atomic charge distribution, frontier molecular orbital analysis and natural bond orbital analysis have been studied by DFT calculation. The natural bond orbital analysis was carried out to interpret hyper conjugative interaction and intramolecular charge transfer. The frontier molecular orbital analysis shows the pharmaceutical activity of the compound. The antibacterial activity for APZHT compound was screened against human pathogens.

**Research Scholars** 

Mr. K.S. Manoj – Crystal Growth
Ms. K. Nithya - Environmental Materials
Mr. S. Pon lakshmanan - Water splitting

Ms. K. Kaviya – Energy Materials Ms. S. Hemapriya - Supercapacitor Mr. P. Ragul - Supercapacitor



Mr. Sundararajaperumal is now pursuing a Ph.D. under the supervision of Dr. M. Mahendran. His research focuses on two areas: wastewater treatment and green hydrogen production, both of which are crucial in terms sustainable development and environmental preservation. In barely 2.5 years of PhD study, he has shown extraordinary academic productivity and research commitment. He has successfully published five research peer-reviewed papers reputable, international publications, demonstrating his high research aptitude. In addition to these articles, he has submitted two further manuscripts, which are now being reviewed. His steady production demonstrates both the scientific excellence and the significance of his research activity. He was technical expertise includes working with sputtering systems, a vital tool in thin-film deposition that is widely employed in material science and nanotechnology.



Name: A. Anusuya

Qualification: M. Sc., M.Phil.,

B.Ed.

Position: Ph.D. Scholar (Full-Time)

Fellowship: Thiagarajar Research

Fellowship

Supervisor: Dr. S. Karthickprabhu

PhD Thesis: Supercapacitors
Date of Joining: 05.01.2024



Name : P. Sundararajaperumal

Qualification: M. Sc (MKU)

Position: Ph.D Scholar (Full-Time)

Fellowship: Thiagarajar Research

Fellowship

Supervisor : Dr. M. Mahendran PhD Thesis : Waste Water Treatment

and Green Hydrogen Production

Date of Joining : 02.01.2023

Ms. A. Anusuya, an emerging researcher in the field of energy storage, has consistently excelled both academically and in research. She is a gold medalist in S.S.L.C., securing a perfect score in Mathematics and a state second rank in Tamil, and also a college topper in M.Sc. Physics. Demonstrating a commitment to continuous learning, she has earned verified certificates from top global institutions: Her doctoral research focuses on highperformance materials for supercapacitors. She has authored several research papers, including: "Architecting Copper-Based Mono- to Multi-Metallic MOFs: A Pathway to High-Performance Supercapacitor Electrodes" (under peer review), "Revealing the Structural and Electrochemical Characteristics of Bimetallic MnCo<sub>2</sub>O<sub>4</sub> Nanoparticles as High-Performance Hybrid Supercapacitor Electrodes" (accepted in a Scopusindexed conference), and "The Transformative Role of Nano-SiO<sub>2</sub> in Polymer Electrolytes for Enhanced Energy Storage Solutions" (published).

Ms. C. Thirisha, Currently researching quantum computing for healthcare applications, she explores how Quantum mechanical principles like superposition and entanglement can enhance diagnostic accuracy using Variational Quantum Eigensolver (VQE) and Quantum Approximation Optimization Algorithm (QAOA). In her first year, she submitted two research papers to International reputed journals and won Best Paper Awards at SRM's "ICFMST" and Thiagarajar College of Engineering's Research Conclave. Proficient in Python and Qiskit, she designs quantum circuits to analyse complex systems. Her post-graduation work focused on optimizing microstrip patch antennas. Academically, she holds a First Class with Distinction in UG and First Class in PG. She actively engages in co-curricular securing prizes in quizzes.



Name: C. Thirisha

Qualification: M. Sc (MKU)

Position: Ph.D. Scholar (Full-Time)

Fellowship: Thiagarajar Research

Fellowship

Supervisor: Dr. M. Mahendran PhD Thesis: Quantum Computing

Date of Joining: 18.07.2024



Name: M. Deepikaa

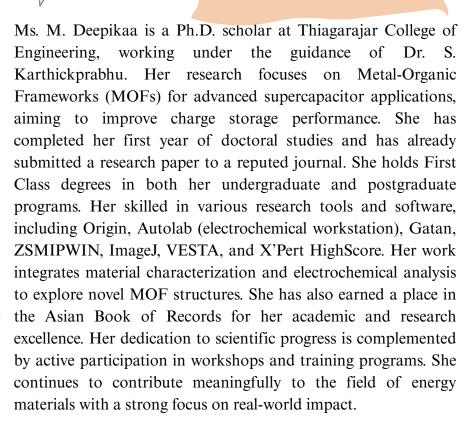
Qualification: M. Sc (M KU)

Position: Ph.D Scholar (Full-Time) Fellowship: Thiagarajar Research

Fellowship

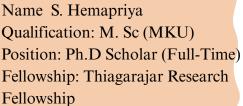
Supervisor: Dr. S. Karthickprabhu

PhD Thesis: Supercapacitor Date of Joining: 24.07.2024



I am currently engaged in research on supercapacitor applications under the guidance of Dr. M. Mahendran. My work focuses on the development of efficient electrode materials and their electrochemical performance for energy storage systems. As part of this ongoing research, I have published one paper in a peer-reviewed journal and have submitted another manuscript that is presently under review. In recognition of my contributions, I have received two Best Paper Presentation Awards at international conferences, which reflect the quality and impact of my research. This experience has strengthened my expertise in materials characterization, device fabrication, and scientific communication within the field of energy storage.





Supervisor: Dr. P. Velusamy PhD.Thesis: Energy&

Environmental Application Date of Joining: 24.07.2024





Name: K. Aruna Devi Qualification: M. Sc (MKU) Position: Ph.D Scholar (Full-Time)

Fellowship: Thiagarajar Research

Fellowship

Supervisor: Dr. M. Mahendran

PhD. Thesis: Energy & Environmental application

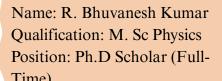
(Supercapacitor)

Date of Joining: 24.07.2024

Hema Priya is a passionate research scholar focused on energy innovation and environmental sustainability. Her academic began with standout M.Sc. thesis journey a "GQDs/Fe<sub>3</sub>O<sub>4</sub>/Ppy Electrocatalysts for Creatinine Sensing," which earned her an international conference presentation in Madurai. She received a TNSCST-funded research grant for developing Ag-doped CuS nanoparticles using neem extract for eco-friendly agricultural applications. A former Club Secretary of "Thinkers" and Placement Representative, she helped 15 classmates secure jobs and was honored as the Best Outgoing Student at Thiagarajar College of Arts & Science. Proficient in research tools like Origin, ImageJ, Fityk, and ZSimpwin, she is also known for her aesthetic scientific presentations. Her recent publications include studies on Co3+-doped TiO<sub>2</sub>/MnWO<sub>4</sub> nanocomposites (Inorganic Chemistry Communications) and NiFe<sub>2</sub>O<sub>4</sub>/NiO/g-C<sub>3</sub>N<sub>4</sub> electrocatalysts for (Diamond & Related Materials), underscoring her commitment to sustainable nanomaterial solutions.

Kaviya K completed her undergraduate degree in Physics at The Standard Fireworks Rajaratnam College for Women with First Rank. She pursued her postgraduate studies at Ayya Nadar Janaki Ammal College, securing a Gold Medal for academic excellence. During her PG studies, she completed an internship at Madurai Kamaraj University, where she gained handson experience in nanomaterials research. Currently, she is a research scholar at Thiagarajar College of Engineering, working under the guidance of Dr. M. Tamilelakkiya. Her doctoral research is centered on materials science, with a focus on electrocatalysis and photocatalysis.



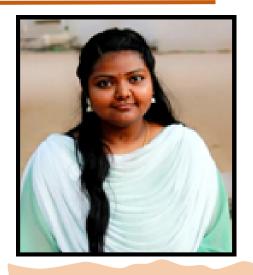


Fellowship: Thiagarajar Research

Fellowship

Supervisor: Dr. M. Mahendren PhD Thesis: Bismuth-based Nanomaterials for Energy. Date of Joining: 24.07.2024





Name : Kaviya K

Qualification : M. Sc Physics

Position: Ph.D Scholar (Full-Time) Fellowship: Thiagarajar Research

Fellowship

Supervisor : Dr. M. Tamilelakkiya

PhD Thesis: Nanomaterials for

Energy Applications

Date of Joining : 30.07.2024

In the pursuit of sustainable technological solutions, R. Bhuvanesh Kumar, advanced research on the development of photocatalytic and electrocatalytic materials for energy and environmental applications. His current work focuses on material design strategies such as doping and nanostructure engineering to enhance catalytic performance in processes like water splitting and pollutant degradation. Within the first year of his doctoral studies, he submitted a conference research article to a reputed journal, Technically adept in material synthesis and characterization methods—including hydrothermal synthesis, XRD, SEM, UV-Vis, XPS, and proficient handling of the electrochemical workstation—he brings a hands-on, analytical approach to experimental science. Academically, Bhuvanesh Kumar has demonstrated consistent excellence. securing First Class undergraduate studies and earning Second Rank in his postgraduate program.

Mr. Manoj K.S has completed his Bachelors degree from Mahatma Gandhi University, Kottayam. During his B.Sc degree he has participated on solar cell making workshop conducted by IIT Bombay. He completed his M.Sc from Madurai Kamraj University, Madurai. As an excellence of his leadership he has organized intercollege meet and national science day events during his master's degree. Now he is pursuing his research in Crystal growth for Non Linear Optical Applications under the guidance of Dr. M. Tamilelakkiya. He has been awarded best poster presentation award at "National Symposium on Recent Advances in Electrical, Optical and Magnetic Materials" held at Karpagam Academy of Higher education Coimbatore. He has submitted his research work on reputed journals.



Name: M. Nandha Kumar Qualification: M.Sc., M. Phil.,

B.Ed.,

Position:Full-Time Research Scholar

Fellowship: Thiagarajar Research

Fellowship

Supervisor: Dr.M.Mahendran Thesis: Thermoelectric Heusler

Alloys

Date: 12.08.2024





Name: Manoj K.S

Qualification: M. Sc (MKU)

Position: Ph.D Scholar (Full-Time) Fellowship: Thiagarajar Research

Fellowship

Supervisor: Dr. M. Tamilelakkiya

PhD Thesis: Crystal Growth Date of Joining: 30.07.2024

He is a full-time Research Scholar in the Department of Physics at TCE, having joined in July 2024. His research area lies in computational physics with specialization in Density Theory (DFT) simulations, Functional focusing multiferroic materials, thermoelectric systems, and solar cell materials. He completed his B.Sc. and M.Sc. in Physics from The Madura College, graduating with First Class in both degrees. He also holds a B.Ed. from Tamil Nadu Teacher's University and an M.Phil. in Physics from Madurai Kamaraj University, where he secured First Class with Distinction. He has teaching experience at various schools and research experience as a Project Fellow in a UGC-sponsored project, which strengthened his interest in physics research and academics. From 2019 to 2025, he has published three research papers, including two as a co-author and one as the first author in a Q1-ranked journal. His goal is to contribute significantly to the field of computational materials science through high-quality research and publications.

Like a Photon that dances through space carrying energy and light, brings a quiet spark of intelligence into every step of her academic journey. She is a research scholar in computational material science, focuses her work on Density Functional Theory (DFT) and Device Simulations. She published her First Q2 journal article titled "Numerical Simulations of the Efficiency of BiFeO<sub>3</sub> Perovskite Solar Cells" and received Best Paper Award at "ICFMST-2024" organized by SRM TRP, Trichy. Eager to broaden her academic exposure, she participated in several conferences and workshops, including ANEH-2024 (Dindigul), ICOLD'25 (IIT Hyderabad), and QST PU 2025 (Pondicherry). Even before her research life began, During her PG and UG, she won 2nd and 3rd prizes in Telegenic Lectures at "Aperion 2023 & 2024" (Bharathidasan University), 1st prize in a semiconductor-themed dance at Galaxon'24 (Madura College) and Best Poster. She was also honored as the Best Performer Award by the Naandi Foundation. She completed her both degree with First Class. Reema's journey moves from small steps to shining milestones quietly powerful and full of potential.



Name: S. Pon Lakshmanan

Qualification: M. Sc., (Manonmaniam

sundaranar University)

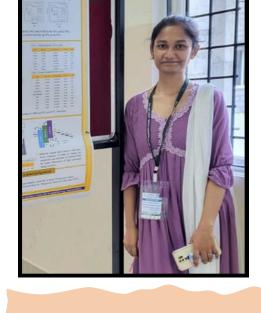
Position: Ph.D Scholar (Full-Time) Fellowship: Thiagarajar Research

Fellowship

Supervisor : Dr. P. Velusamy

Ph.D. Thesis: Energy and Environmental

Application (Water Splitting)
Date of Joining: 03.09.2025



Name: S. Reema Sagitha Qualification: M.Sc Physics

Position : Doctor of Philosophy Fellowship : Thiagarajar Research

Fellowship

Supervisor : Dr. V. Aravindan Ph.D. Thesis : Computational

Material Science

Date of Joining: 14.08.2024



He is currently pursuing his Ph.D. under the guidance of Dr. P. Velusamy, with a research focus on water splitting. He has published two research papers in reputed journals and was honoured with the Best Oral Presentation Award at an international conference. In addition, he actively participated in speech and debate competitions as part of the longest multinational confluence, spanning over 2,600 hours, organized by the Assist World Record Foundation.

A passionate Ph.D. scholar at Thiagarajar College of Engineering, Madurai, is making strides in the field of Ion Beam Irradiation under the mentorship of Dr. P. Sivakumar. Having joined the program on January 31, 2025, this researcher brings strong academic credentials, including an M.Sc. in Physics with First Class from Madurai Kamaraj University. Awarded the Thiagarajar Research Fellowship, they have shown remarkable promise in experimental material science. Their research focuses on understanding ion interactions with advanced and functional materials. They have also demonstrated excellence outside the lab, winning multiple quiz competitions. Discipline and determination define their approach to research. Their work bridges theoretical concepts with real-world applications. Peers admire their consistency and leadership in academic settings.





Qualification: M. Sc (Bharathidasan

University)

Position: Ph.D Scholar (Full-Time)

Fellowship: Thiagarajar Research

Fellowship

Supervisor: Dr. P. Velusamy

PhD Thesis: Energy storage, Water splitting, and Dye degradation Date of Joining: 03/02/2025



Name: Pretika PA

Qualification: M. Sc (Madurai

Kamaraj University

Position: Ph.D. Scholar (Full-Time)

Fellowship: Thiagarajar Research

Fellowship

Supervisor : Dr. P. Sivakumar PhD Thesis : Ion beam irradiation

Date of Joining: 31/01/2025

He is a Ph.D. scholar specializing in sustainable energy storage, water splitting, and dve degradation. His research focuses on designing advanced nanomaterials and photocatalysts to improve battery and supercapacitor performance, develop efficient electrocatalysts for hydrogen production, and remove toxic dyes wastewater. Through interdisciplinary approaches, he aims to advance clean energy solutions and promote environmental sustainability.

Nithya is a Physics research scholar currently pursuing her Ph.D. at Thiagarajar College of Engineering under the guidance of Dr. M. Tamilelakkiya. She completed her B.Sc. at V.V.V. College for Women, Virudhunagar, and her M.Sc. at V.H.N.S.N. College, Virudhunagar. She also holds an M.Phil. from Madurai Kamaraj University and a B.Ed. from Sri Vasta College of Education. Her research focuses on nanomaterials, particularly for water splitting applications aimed at clean energy solutions. She is interested in understanding how nanoscale materials can contribute to addressing global energy needs.





Name: K. Nithya

Qualification: M. Phil (MKU)
Position: Ph.D Scholar (Full-Time)
Fellowship: Thiagarajar Research

Fellowship

Supervisor : Dr. M. Tamilelakkiya PhD Thesis : Nanomaterials for

**Energy Applications** 

Date of Joining: 01/03/2025



S. SIVA PRAKASH SUPPORTING STAFF

#### **NEW QUANTAS**



B. PRABHU



R.K.JITHESH



P.NIVETHA

#### **RESEARCH INTERNSHIP**

A two-week internship program titled "Internship opportunity for UG/PG students" was conducted by Department of Physics at Thiagarajar College of Engineering during July 2025. The aim of the internship was to provide hands-on training and research exposure in cutting-edge areas of physics. This initiative aligns with the department's ongoing mission to promote experiential learning, skill development and academic research culture among students from diverse fields.



#### **Objectives of the Internship**

- To provide practical exposure to advanced physics experiments
- To introduce students to research methodologies and scientific problem-solving.
- To enhance interdisciplinary collaboration among students from various academic backgrounds
- To strengthen core concepts through lab-based learning and project development
- To support student career development via faculty mentorship and guided research.

#### **Areas of Research**

Students were assigned to specialized research themes based on their interests and mentor guidance. The following key areas were covered and the works related to the following fields were assigned to the student interns.

- Thin Films and Coatings: (Sputtering, Spin coating and characterization using UV-VIS)
- Energy Materials: (Material for solar cells, super capacitors, and batteries)
- **Hydrogen Production :** (Photocatalysis, water-splitting electrodes, and electrochemical cells)
- Crystal Growth and Characterization: (Single and polycrystalline growth, microscopy, and structural analysis)
- Computational Simulation: (Software used: COSMOL Multiphysics, SCAPS, VASP, etc.)
- Each student engaged in active project work, laboratory procedures and a final report submission to demonstrate their understanding.

#### **Key Outcomes**

There were 38 students from various colleges who joined as research interns, they successfully completed their research internships and submitted their project reports to their assigned mentors. Students gained practical research experience and had hands-on training in instrumentation and data analysis techniques. They strengthened their interdisciplinary skills and developed collaboration with their mentors and the respective laboratories.

#### **Conclusion**

This internship program was a resounding success, reflecting the Department of Physics of TCE with a commitment to nurture young minds through research and experimentation. The student interns demonstrated commendable enthusiasm and discipline throughout the course, and the skills acquired will make a meaningful contribution to their academic and professional pursuits.

#### 66

### NATIONAL SCIENCE DAY

#### **National Science Day-Symposium**

The Department of Physics organized a one-day symposium on National Science day 2025, to commemorate the remarkable contributions of Dr. C. V. Raman. The theme of the symbosium is on "Empowering Indian youth for Global leadership in Science and Innovation for Viksit Bharat". The main aim of the symposium is to inspire and educate first year graduate students from engineering and science streams about the recent advancements in science and technology to foster a spirit of inquiry and innovation in science. The event provided a platform for young minds to explore, discuss and showcase their scientific innovations. Participants explored diverse and contemporary scientific topics including Fuel for Tomorrow, sustainable E-Wasteb solution, Quantum Computing for the future, A device that can change the world and Novel materials for Engineering innovations. A total of 140 students from various fields participated in the symposium. The symposium featured various competitions including working models, poster presentation and Quiz Fiesta. Dr. M. Mahendran, Head of the department of Physics served as the convener and Dr. V. Aravindan, assistant professor of physics acted as the coordinator of this program The event commenced at 9. 15 a.m at K. S. Auditorium with a welcome address by the coordinator.

#### **66 EVENT INAUGRATION**

The keynote address was given by Prof. M. Mahendran, head of Department of Physics. He gave wonderful talk by highlighting how ancient civilizations intuitively applied fundamental physics principles before they were formally recognized in modern science. The session concluded by emphasizing the contemporary scientific advancements and its deep roots in ancient wisdom, inspiring the attendesc to explore the interdisciplinary nature of Science. This session successfully bridged the gap between historical knowledge and modern physics, fostering curiosity and deeper scientific inquiry. The Presidential address was delivered by Prof. L. Ashok Kumar, Principal and Head of the institution. His speech drew insightful connections between ancient Tamil wisdom and Modern scientific thought with a special focus on Bavanandhi Munivar's Nanool.







#### **EVENTS AND ACTIVITIES**



#### Quiz - Festa

A quiz program was conducted at K. S. Auditorium, Dr. S. Pethuraj, Assistant Professor of Physics conducted the program along with Mr. M. Nandha Kumar and Ms. C. Thrisha, Research Scholars of department of Physics. The quiz featured 45 questions from various domains of Physics. In the first round participants were given 60 seconds to answer each question. The second round followed a rapid-fire format, challenging participants with quick thinking responses.

#### **Poster Presentation**

A poster presentation was held at Physics practical lab were posters and working models were presented. Dr. K. Hariharan, Dr. S. Julius Fusic and Ms. C. V. Nisha Angeline served as jury members for this event. The participants impressed the jury and faculty members with their insightful presentation on quantum computing for the future.

The event got concluded with a valedictory session were prizes were distributed for the winners. Awards for the winners of all events were presented by the Head of the department and program coordinator. The symposium was resounding success, fostering a spirit of inquiry, innovation and knowledge among young students. The enthusiastic participation of students, faculies and research scholars created an intellectually stimulating environment

### INSPIRE MANAK AWARD

The INSPIRE MANAK (Innovation in Science Pursuit for Inspired Research-Million Minds Augmenting National Aspirations and Knowledge) State level Exhibition and Project competition was held on 23<sup>rd</sup> and 24<sup>th</sup> February 2024 at Thiagarajar College of Engineering. Dr. M. Mahendran, Professor and Head, Department of Physics served as the local coordinator.



This program was jointly organized by Department of Science and Technology, New Delhi, National Innovation Foundation, Gujarat and Tamilnadu Science and Technology centre, Chennai. This is a National program which has been implemented for attracting talent among students to study and pursue career in science and research. School students from 6<sup>th</sup> to 10<sup>th</sup> grade are being identified for inspire award. The inauguration of the INSPIRE held on 24.02.2024 at 9:30 am. Dr. M. Palaninatharaja Prinicipal-in-charge, Thiagarajar College of Engineering, Madurai, Thiru.I. K. Lenin Tamilkovan, Executive Director, Tamilnadu Science and Technology Centre, Thiru. N.S. Chidambaram, INSPIRE Coordinator, Tamilnadu Science and Technology Centre, Chennai, Dr. M. Mahendran, INSPIRE Local Coordinator and two NIF representatives chaired the Dias. The function began with the prayer song and kalaithandhai vazhthu. It is followed by the lighting of the kuthuvilaku by the dignitaries on the Dias and two student representatives. The expo began followed by kuthuvilaku lighting.





The program was concluded with a valedictory function, Thiru.I. K. Lenin Tamilkovan, Executive Director, Tamilnadu Science and Technology Centre welcomed the gathering. Palaninatharaja, Prinicipal-in-charge, Thiagarajar College of Engineering, Madurai delivered the chief guest address. The dignitaries were honoured with a memento and a shawl. Thiru. N.S. Chidambaram, INSPIRE Coordinator presented the Report on the Programme, INSPIRE. The INSPIRE team honoured the Jury of TCE. The **INSPIRE** presented the prizes certificates to the winners of the event. Dr. M. Mahendran, Prof & Head of Physics, TCE and INSPIRE Local Coordinator proposed the vote of thanks.

The participants came on February 24, 2024, and set up their projects in the designated locations. 70 students who have been selected from various districts all over Tamilnadu participated in this state level INSPIRE- MANAK Program. The faculty members from various departments of Thiagarajar Engineering college acted as judges for the projects prepared by students. Eight best awardees were selected from the participant depending their on projects meticulously evaluating each project based on originality, scientific relevance, societal impact, and presentation skills. Their expertise ensured a fair and insightful assessment of the students' work. These awardees are eligible for the forthcoming 11th National level exhibition and project competition which is scheduled to be conducted at New Delhi.







### **OLYMPIAD**



The Department of Physics of Thaigarajar College of Engineering organized physics Olymbiad 2024-25 to ignite and nurture enthusiasm for physics among undergraduate engineering students. This intiatives aimed to test their conceptual understanding, analytical skills and problem solving abilities through a series of rigorous and engaging competitions. A total of 204 students participated in this olympiad from various streams of Engineering among these participants 167 students were from I years, 28 students from II year and 9 students from III year. This Olympiad was organized by Dr. V. Aravindan and Dr. P. sivakumar, Assistant Professors of Department of Physics. The students showcased vibrant participation in the Olympiad with great enthusiasm and curiosity which really acted catalyst for deepening understanding in various fields of physics.

#### **OBJECTIVES**

- To evaluate student's knowledge in Engineering Physics through multiple competitive rounds
- To promote scientific thinking, logic and analytical reasoning
- To identify top physics talents from engineering streams
- To inspire them about the importance of understanding basic physics
- To encourage active learning beyond the classroom curriculum.



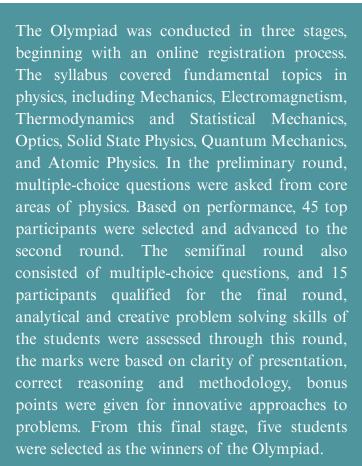
# PRIZE DISTRIBUTION CERP DEPARTMENTS OF MATHEMATICS ACCURATE VARIABLE Thiruparankundram, Tamil Nadu, India TCL Avain-provision flood, Thisperials College of Engineering, Thiruparankundram, Tamil Nadu Sci St. Status Lat 9 882396, Loon 27 00 83716 Note: Captured by GPS Mag Canners







#### **EVENTS AND DESCRIPTION**



#### The top five performers of the Olympiad

I - Z. Syed Zubair Muhammed (I Mech – B)

II - E. S. Fritwin Reo (I ECE-C)

III - T. Athiyamaan

IV - R. Meenashwaran (II CSE-A)

V - P. Sivaprakash (I CSE-C)



Certificates were awarded to all participants in recognition of their involvement. Cash prizes were distributed to the top 45 performers as a token of appreciation for their excellence. The winners were also given the opportunity to attend advanced workshops and conferences, providing them with further exposure to cutting-edge developments in physics and fostering continued academic growth.

### FAGULTY/DEVELOPMENT PROGRAM

A six-day faculty development program was conducted by Department of Physics of Thiagarajar Engineering College on "Recent Trends in Crystal Growth and Applications in collaboration with Indian Association for Crystal growth. The convener of the FDP was Dr. M. Mahendran, Head, Department of Physics and the coordinators were Dr. M. Tamilelakkiya and Dr. P. Sivakumar, Assistant Professors of Department of Physics. Energy harvesting and Conversion, Nonlinear Optical (NLO) materials, controlling crystal defects and Eco-friendly crystal growth techniques were considered as the theme areas of this FDP program.

#### ABOUT THE FDP

This online FDP was conducted for about six days with two to three sessions for each day. Each sessions were handled by experts from various fields.

#### DAY - I

#### Session -I:

The first session was handled by Prof. Ramasamy, President of Indian Association for crystal growth (IACG), SSN Research Centre, Chennai on Silicon ingots grown by India-made DS furnaces, @SSN, 15Kg &800Kg.

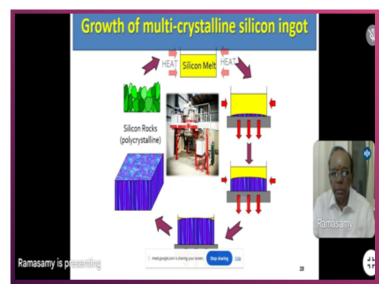
#### Session –II:

Second session was handled by Dr. S. Ganesamoorthy, Scientific Officer-G, IGCAR on Single Crystal for Radiation Detection, Imaging & Transducer Application.

#### DAY - II

#### Session -I:

The first session of the second day was handled by Dr. B. Sridhar, Senior Principal Scientist, CSIR, Hyderabad on X-Ray Crystallography.





#### Session –II:

The second session was handled by Prof. S. Brahadeeswararn, Professor & Head, Anna University, BIT, Trichy on A materials Perspective on organic NLO single crystals for efficient generation and detection of Terahertz waves.

#### DAY - III

#### Session -I:

The first session of the third day was presented by Prof. Binay Kumar, Senior Professor, University of Delhi on Growth and characterization Techniques of Crystal and Energy harvesting applications of piezoelectric crystals/nanoparticles.

#### Session \_II:

The second session of third day was handled by Prof. R. Ramesh Babu, Head, Department of Physics, Bharathidasan university on Advances in Bulk Growth of Organic Nonlinear Optical Single Crystals using Vertical Bridgman and Gradient Freeze Methods.

#### DAY-IV

#### Session -I:

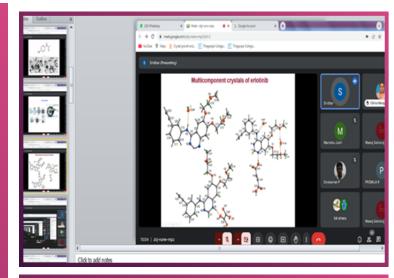
The first session of the fourth day was presented by Prof. K. Sethuraman, Professor, Central University, Tamilnadu.

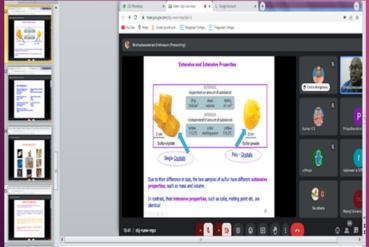
#### Session –II:

The second session of the fourth day was presented by Prof. S. Moorthy Babu, Professor, Anna University, Chennai on Crystal growth of OXIDES for Strategic Applications.

#### Session -III:

The speaker for the third session of the fourth day was Prof. R. Thagavel, Associate Professor, IIT Dhanbad.









#### DAY - V

#### Session -I:

The first session of fifth day was presented by Dr. P. Samuel, Associate Professor, VIT, Vellore on Recent Trends in Laser Physics.

#### Session –II:

The second session of fifth day was presented by Dr. R. Nagalakshmi, Associate Professor, NIT, Trichy on Crystalline materials for optical and cooling applications.

Session –III: Q-AATRA

The speaker for the third session of the fifth day was

Dr. K. Sankaranarayanan, Senior Professor and

Head, Alagappa University on Development of

Unidirectional Organic Scintillator Crystals.

#### DAY - VI

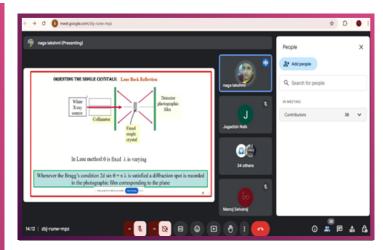
#### Session -I:

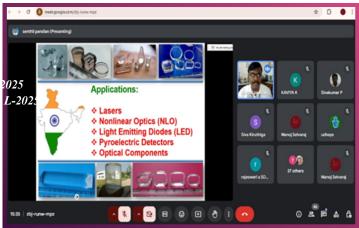
The first session of sixth day was presented by Dr. Muthu Senthil Pandian, Research Scientist, SSN Research Centre, Chennai on Development of High Quality Single Crystals by Unidirectional Solution Methods.

#### Session –II:

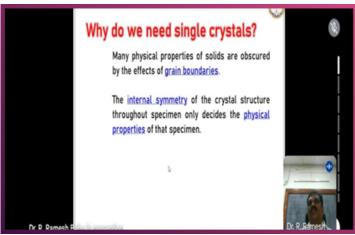
The second session of sixth day was presented by Dr. R. Arun Kumar, Associate Professor, NIT, Trichy on Single crystals for luminescence and dosimetry applications.

The FDP was concluded with a valedictory section marking the successful conclusion of a week filled with academic enrichment and collaborative learning. The session was graced by distinguished speakers, faculty members, and participants from various institutions, all of whom reflected on the insights gained and the impact of the program. This FDP was highly informative which









covered various fields on Recent growth of Crystals and Applications. This FDP proved to be highly informative and intellectually stimulating, offering a comprehensive exploration of the recent advancements in crystal growth and its multifaceted applications. The sessions were meticulously curated to cover both theoretical foundations and practical innovations, making it a valuable experience for researchers and academicians.





Inauguration of the Centre of Excellence in Materials Research and Energy Solutions (COEMRES),

Official Website Launch of MQUBDT'26

International Conference on Materials for Electronics, Energy, Quantum, and Biomedical Technologies & Workshop & Hands-on Training: "Energy Storage Materials" Aug 20 2025

Workshop & Hands-on Training: Fundamentals and Practice of Rietveld Refinement using X-ray Diffraction Data Aug 25-26 **2025** 

Workshop & Hands-on Training: "Quantum Computing" Sep 10 2025

80

## upcoming EVENTS



Workshop: "Electrochemical Techniques for Energy Applications" Sep

17

2025

FDP: "Smart Magnetic Materials: Enabling Technologies for Intelligent Devices" Sep

24

2025

FDP: "Novel Functional Materials and their role in emerging technologies" Dec

01

2025

Hands-on Training: "Computational Tools for Materials Modelling and Simulation" Nov

19

2025

Q-AATRAL-2025

# upcoming EVENTS



Hands-on Training: "Electrochemical Workstation for Students and Faculties" Dec

18

2025

FDP: "Frontiers in Sensor Materials and Sustainable Energy Solutions" Feb

12

2026

FDP: Emerging trends in Biomaterials, Materials design, and simulation techniques Feb

19

2026

International Conference: on "Materials for Electronics, Energy, Quantum and Biomedical Techniques (MQUBIT 2026) (Pre-Conference Workshop)

Mar

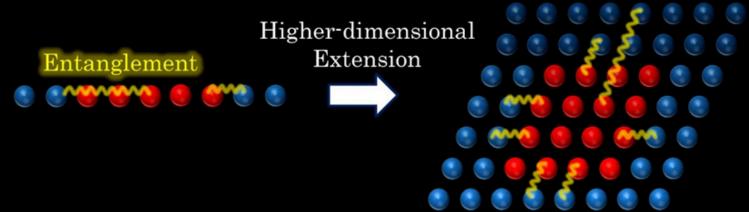
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2026

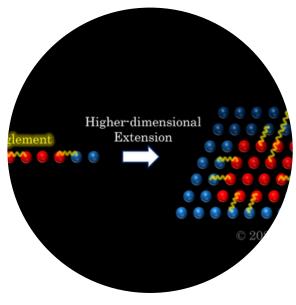
Q-AATRAL-2025

### Physics - Streaming Now..

PHYS.ORG 06 August,2025



### Researchers discover universal rules of suki quantum entanglement across all dimensions



by, <u>The Kavli Foundation</u>,

> edited by, <u>Sadie Harley</u>,

> reviewed by, <u>Robert Egan</u>

### Researchers discover universal rules of quantum entanglement across all dimensions

A team of theoretical researchers used thermal effective theory to demonstrate that quantum entanglement follows universal rules across all dimensions. Their study was <u>published</u> online in Physical Review Letters.

"This study is the first example of applying thermal effective theory to quantum information. The results of this study usefulness demonstrate the ofthis approach, and we hope to further develop approach to gain a understanding of quantum entanglement structures," said lead author and Kyushu University Institute for Advanced Study Associate Professor Yuya Kusuki.

#### PHYS.ORG

07 August, 2025

# DIRECT VISUALIZATION OF QUANTUM ZERO-POINT MOTION IN COMPLEX MOLECULE REVEALS ETERNAL DANCE OF ATOMS

For a long time patterned zero-point movements were considered impossible to measure directly. However, scientists at Goethe University Frankfurt and partner institutions have now succeeded in doing precisely that at the world's largest X-ray laser, the European XFEL in Hamburg, Germany.

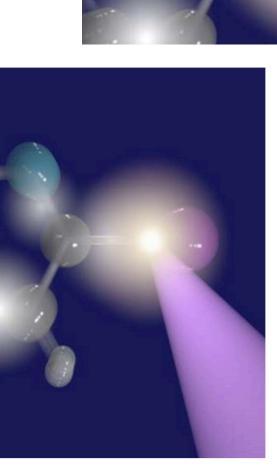
They captured the "dance of the atoms" by shining a "spotlight" on individual molecules and taking snapshots of their atoms—revealing each atom's precise choreography.

Professor Till Jahnke from the Institute for Nuclear Physics at Goethe University Frankfurt and the Max Planck Institute for Nuclear Physics in Heidelberg explains,"The exciting thing about Our work is that we were able to see that the atoms don't just vibrate individually, but that they vibrate in a coupled manner, following fixed patterns.

by,
Goethe University Frankfurt am Main

edited by,
Stephanie Baum,

reviewed by, Robert Egan



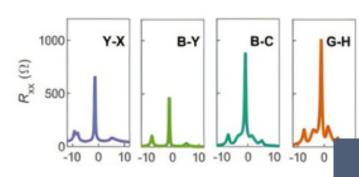
07 ,August 2025

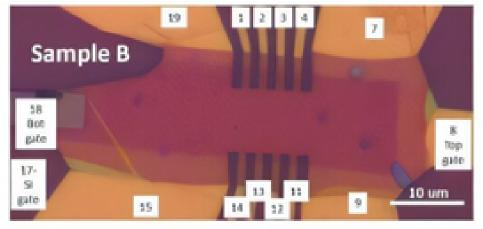
### Researchers overcome long-standing bottleneck

### SINGLE PHOTON DETECTION WITH TWISTED 2D MATERIALS

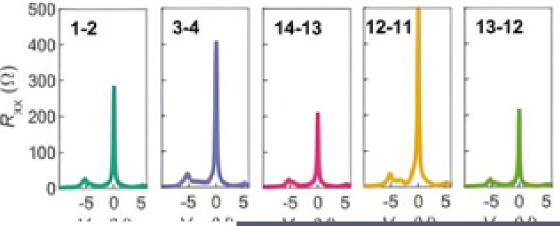
The ability to detect single photons (the smallest energy packets constituting electromagnetic radiation) in the infrared range has become a pressing need across numerous fields, from medical imaging and astrophysics to emerging quantum technologies. In observational astronomy, for example, the light from distant celestial objects can be extremely faint and require exceptional sensitivity in the mid-infrared.







An international team of researchers led by ICFO has now shown one way to overcome this limitation. They have used two-dimensional materials (which are only one-atom thick) to detect long-wavelength single photons (up to the midinfrared) at relatively high temperatures (around 25 degrees Kelvin). This milestone has caught the attention of the European Space Agency (ESA), which is seeking the use of detectors with these types of properties for space exploration.



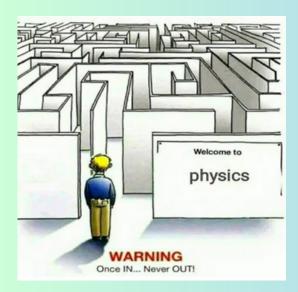
by, <u>ICFO</u>,

edited by,
<a href="mailto:StephanieBaum">StephanieBaum</a>,

reviewed by,

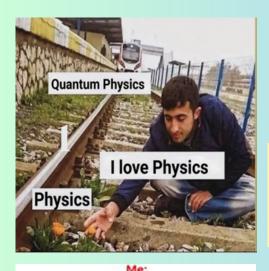
Andrew Zinin

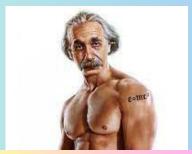
### Fun with Physics



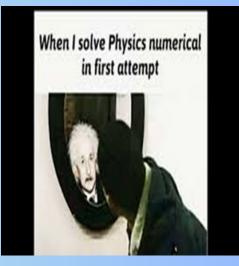




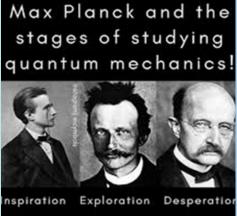


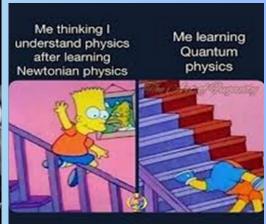


I fear the day that technology will surpass our human interaction. The world will have a generation of idiots



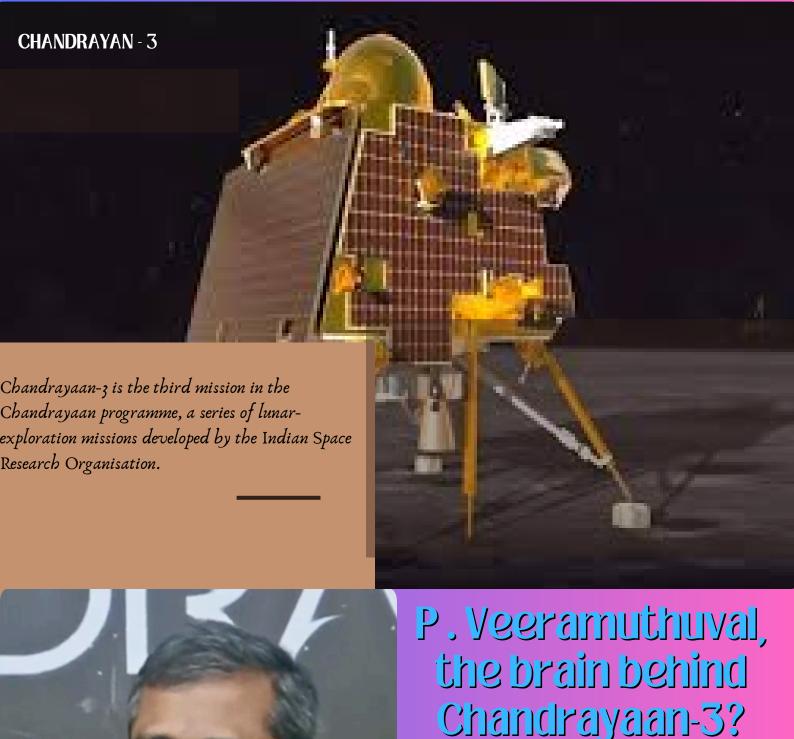






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## Chandrayaan-3?

As India became the first country to land a probe near the south pole region of the Moon on August 23, one man, who has been at the centre of all the limelight is Chandrayaan 3 mission director P Veeramuthuval. Born in Tamil Nadu's Viluppuram district in 1976, Veeramuthuvel had a middleclass upbringing. His father worked as a technician in Indian

He did his schooling at the railway school in Villupuram and then earned a diploma in mechanical engineering from a local polytechnic college. After the mechanical engineering diploma, Veerumuthuvel, who has been living the dream of being a scientist at the Indian Space Research Foundation (ISRO) since childhood, went to a private college to complete his bachelor's degree in engineering. From there, he went to NIT Trichy for his Master of Engineering studies.

