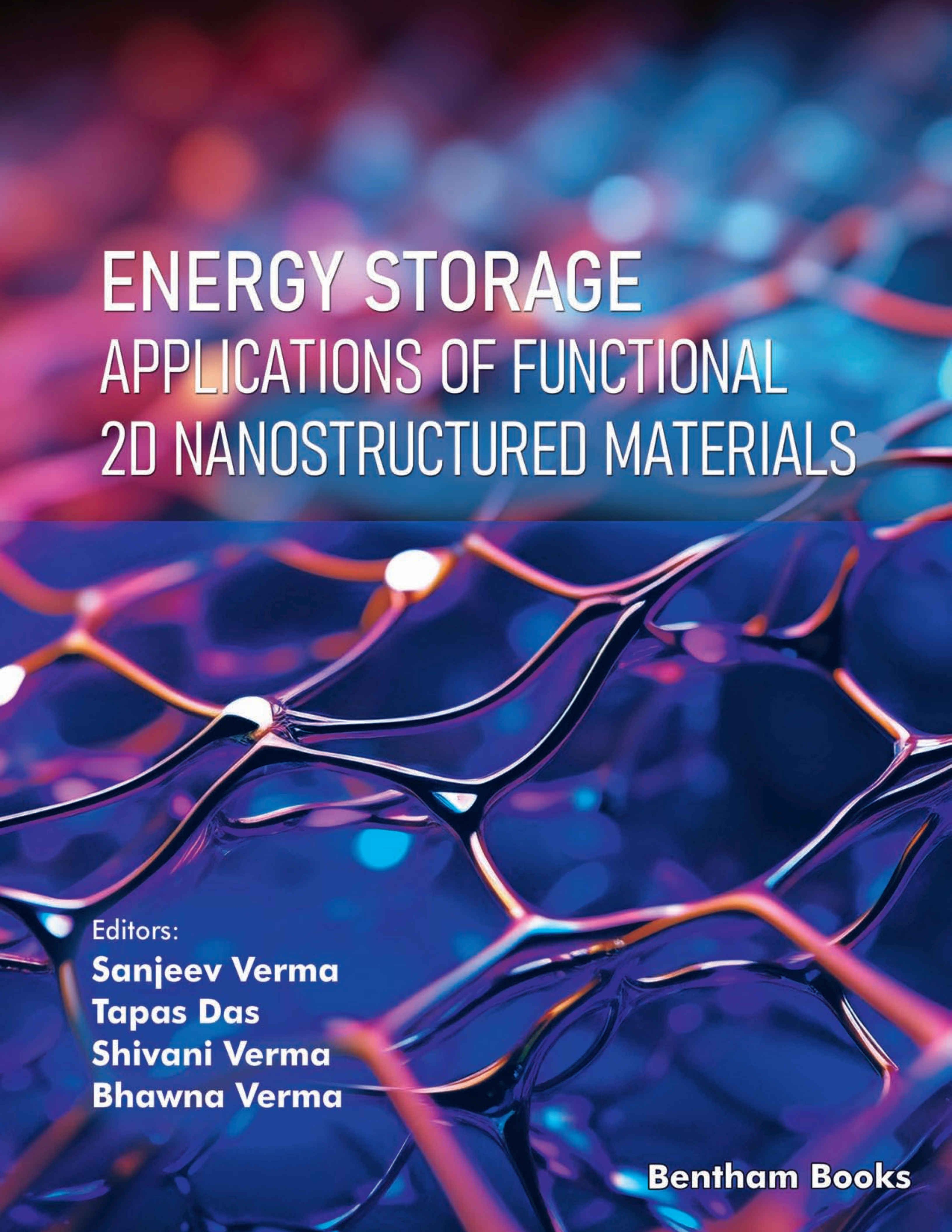

ENERGY STORAGE APPLICATIONS OF FUNCTIONAL 2D NANOSTRUCTURED MATERIALS

Editors:
Sanjeev Verma
Tapas Das
Shivani Verma
Bhawna Verma

Bentham Books

Energy Storage Applications of Functional 2D Nanostructured Materials

Edited by

Sanjeev Verma
Department of Chemical Science and Technology
National Institute of Technology Patna
Patna-800005, Bihar, India

Tapas Das
Department of Chemical Engineering
National Institute of Technology Rourkela
Rourkela-769008, Odisha, India

Shivani Verma
Department of Chemistry, School of Physical Sciences
Doon University, Dehradun-248012
Uttarakhand, India

&

Bhawna Verma
Department of Chemical Engineering and Technology
Indian Institute of Technology (Banaras Hindu University)
Varanasi-221005, Uttar Pradesh, India

Energy Storage Applications of Functional 2D Nanostructured Materials

Editors: Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma

ISBN (Online): 979-8-89881-636-0

ISBN (Print): 979-8-89881-637-7

ISBN (Paperback): 979-8-89881-638-4

Published by Bentham Science Publishers Pte. Ltd. Singapore, in collaboration with Eureka Conferences, USA.

First published in 2026.

Bentham Science Publishers Pte. Ltd.
No. 9 Raffles Place
Office No. 26-01
Singapore 048619
Singapore
Email: subscriptions@benthamscience.net

CONTENTS

FOREWORD

The generation and storage of sufficient energy have become extremely difficult in the 21 century due to the depletion of fossil fuel resources and environmental concerns. Unquestionably, cutting-edge nanotechnology may be the only way to meet humankind's energy needs in the future by creating a safe, eco-friendly, and sustainable energy source. Functional 2D nanomaterials, such as graphene, MXene, MOFs, COFs, and metal nitrides, have the potential to produce and conserve energy sustainably, as well as to support appropriate energy applications.

The authors have provided a thorough overview of the functional 2D nanostructured materials, including graphene, MXene, MOFs, COFs, and metal nitrides, as well as their respective nanocomposites. Such materials have several great uses for the effective storage of energy, mainly supercapacitor electrochemical energy. These materials have a wide range of uses, including flexible nanocomposites for optical memory, future display technologies, biosensors, and nanodevices. I think this book will be very beneficial to the scientific and engineering community.

It is noteworthy to mention that a number of experts from reputed institutes, who have vast background and expertise in the relevant domain, have also contributed to the book chapters. The book appears to be well edited, consistent in flow, and oriented towards expanding the reader's knowledge.

This book will have significant impact on the topic of using next generation nanomaterials in electronics and supercapacitors for energy storage. Many research teams and industry professionals, including those involved in physics, chemistry, materials science, polymer science, energy conversion, chemical engineering and energy storage materials, will find this book to be very useful.

P.K. Jain
Department of Electronics and Communication Engineering
National Institute of Technology Patna
Patna-800005, Bihar, India

PREFACE

The most significant inventions in the field of energy storage and conversion in today's energy-dependent society are electrochemical devices such as electrochemical supercapacitors (ESs), fuel cells, and batteries. Supercapacitor is the clean energy resources for energy. Clean energy is defined as energy that is produced using renewable, non-polluting, zero-emission resources and includes energy that is conserved through energy-saving practices. The electrochemical supercapacitor often referred to as an electrochemical double-layer capacitor, ultracapacitor, or supercapacitor, is a high-performance capacitor that has a higher energy density than those offered by regular capacitors. The ability to quickly charge, have lengthy charge-discharge cycles, and operate in a wide variety of temperatures are just a few of the high-impact traits that ES devices have. They are so widely used in electronics, aviation, smart grids, hybrid and electrical automobiles, and other transportation systems. ES systems still have significant limitations, like high cost and low energy density, but with continued advancement, ESs will be able to both supplement batteries and fuel cells as a power source and stand-alone high energy storage devices.

Functional two-dimensional (2D) nanoparticles are a major contributor to these materials and are frequently used in energy applications because of their distinctive structure and inexpensive cost. Due to their superior electrochemical characteristics, surface area, ability to integrate with nanodevices, multifunctionality, printability, and mechanical flexibility, functional 2D nanomaterials have become intriguing options for energy devices. Graphene, MXene, transition metal nitrides/chalcogenides, MOFs, and COFs-based functional nanostructured advanced materials for energy applications mainly in supercapacitors, are some of the materials in the 2D category for which we outline research topics in this book.

Additionally, the introduction of electrochemical supercapacitors from a more scientific and practical standpoint as well as their advancement over the previous ten years will be emphasized in our book. It presents the fundamental electrochemical theory and computations and talks about the various parts and characterization methods. The structure and available alternatives for device packing are the topics of further discussion. The book will provide enough technical information on novel active materials synthesized by specialists in the energy field that could develop in future, as well as shed light on the practical elements of comprehending and using the technology in the industry. To further aid readers in understanding the practical limitations and the criteria that go along with them in ES technology, the practical challenges are also explored in this book.

Sanjeev Verma
Department of Chemical Science and Technology
National Institute of Technology Patna
Patna-800005, Bihar, India

Tapas Das
Department of Chemical Engineering
National Institute of Technology Rourkela
Rourkela-769008, Odisha, India

Shivani Verma
Department of Chemistry, School of Physical Sciences
Doon University, Dehradun-248012
Uttarakhand, India

&

Bhawna Verma
Department of Chemical Engineering and Technology
Indian Institute of Technology (Banaras Hindu University)
Varanasi-221005, Uttar Pradesh, India

List of Contributors

Abhinaba Das	Functional Materials Group, Advanced Materials & Corrosion (AMC) Division, CSIR-National Metallurgical Laboratory (NML), Burmamines, East Singhbhum, Jamshedpur, Jharkhand-831007, India
Abhishek Kumar	Department of Chemical Engineering, National Institute of Technology Rourkela, Rourkela-769008, Odisha, India
Abu Jahid Akhtar	Department of Physics, Diamond Harbour Women's University, West Bengal, 743368, India
Arnab Samanta Roy Choudhury	Functional Materials Group, Advanced Materials & Corrosion (AMC) Division, CSIR-National Metallurgical Laboratory (NML), Burmamines, East Singhbhum, Jamshedpur, Jharkhand-831007, India
Arpita Dutta	Department of Physics, Diamond Harbour Women's University, West Bengal, 743368, India
Awadh Kishor Kumar	Department of Chemical Engineering and Technology, National Institute of Technology Patna, Bihar - 800005, India
Badekai Ramachandra Bhat	Catalysis and Materials Chemistry Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, Mangalore 575025, Karnataka, India
Banavath Anil Kumar Naik	Department of Chemical Engineering and Technology, National Institute of Technology Patna, Bihar - 800005, India
Bhawna Verma	Department of Chemical Engineering and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi-221005, India
Challapalli Subrahmanyam	Energy and Environmental Laboratory, Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy 502285, Telangana, India
Chandra Bhal Singh	School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi-221005, India
Dibyananda Majhi	Energy and Environmental Laboratory, Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy 502285, Telangana, India
Dipsikha Ganguly	Mechanical Engineering, National University of Singapore, Singapore
Hara Mohan Jena	Department of Chemical Engineering, National Institute of Technology Rourkela, Rourkela-769008, Odisha, India
Krunal M. Gangawane	Department of Chemical Engineering, Indian Institute of Technology Jodhpur, Jodhpur-342030, Rajasthan, India
Pallab Bhattacharya	Functional Materials Group, Advanced Materials & Corrosion (AMC) Division, CSIR-National Metallurgical Laboratory (NML), Burmamines, East Singhbhum, Jamshedpur, Jharkhand-831007, India Academy of Scientific & Innovative Research (AcSIR), Ghaziabad 201002, India
Ponraj Jenis	Materials Science and Engineering, National University of Singapore, Singapore

Rayavarapu Prasada Rao	Mechanical Engineering, National University of Singapore, Singapore
Satyendra Kumar Satyarthi	School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi-221005, India
Seeram Ramakrishna	Mechanical Engineering, National University of Singapore, Singapore
Shreeganesh Subraya Hegde	Energy and Environmental Laboratory, Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy 502285, Telangana, India Catalysis and Materials Chemistry Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, Mangalore 575025, Karnataka, India
Simi Pushpan K.	Department of Chemistry, Union Christian College, Aluva, Kerala, 683102, India
Sudip Kumar Saha	Department of Physics, Diamond Harbour Women's University, West Bengal, 743368, India
Sunil Kumar Singh	Department of Chemical Engineering, BIT Sindri, Dhanbad, Jharkhand-828123, India
Tapas Das	Department of Chemical Engineering, NIT Rourkela, Odisha-769008, India
Vidhya K. V.	Department of Chemistry, Union Christian College, Aluva, Kerala, 683102, India
Vikas Kumar Pandey	Department of Chemical Engineering and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi-221005, India
Vishwa Pratap Singh	UNAM – National Nanotechnology Research Center and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Türkiye

CHAPTER 1

Introduction to Functional 2D Nanostructured Materials

Awadh Kishor Kumar[1] and **Banavath Anil Kumar Naik**[1,*]

[1] *Department of Chemical Engineering and Technology, National Institute of Technology Patna, Bihar-800005, India*

Abstract: The current market is focused on developing flexible and easily fabricated equipment, particularly in the electronics and automobile industries, where there's growing interest in flexible and wearable devices. These devices require power stored in energy storage devices, but current rigid options, such as coin cells and batteries, are incompatible, causing discomfort. Thus, there is a significant focus on developing flexible energy storage solutions.

Many methodologies have been developed to design nanomaterials for energy applications, focusing on various dimensions, morphologies, and properties. Since the successful exfoliation of graphene from graphite in 2004, two-dimensional nanomaterials have garnered significant attention due to their remarkable features, including a high specific surface area, thermal conductivity, carrier mobility, chemical activity, strength, and tunable electronic properties. These materials, with sheet-like structures larger than 100 nm in lateral size and molecular thickness, exhibit excellent mechanical properties, electronic properties, and light transmittance, making them ideal for next-generation electronic devices. Compared to other nanomaterials such as nanowires, 2D nanomaterials' uniformly exposed lattice plane, and unique electronic state are crucial for energy storage.

The combination of nanomaterials and two-dimensionality creates synergistic effects, enhancing energy application performance. This chapter discusses the advancements of 2D nanomaterials in energy applications, summarizing key points in energy storage and conversion systems, and exploring their uses. It highlights the latest progress of 2D nanomaterials in energy-related functional applications.

Keywords: Boron nanosheets, Energy storage, Graphene, MXene, Nanomaterials, Silicene, Supercapacitors, Top-down approach, Transition metal dichalcogenides, Two-dimensional.

* **Corresponding author Banavath Anil Kumar Naik:** Department of Chemical Engineering and Technology, National Institute of Technology Patna, Bihar - 800005, India; E-mail: banavath.ch@nitp.ac.in

Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma (Eds.)

INTRODUCTION

Nanotechnology represents the forefront of modern material science, focusing on engineering, technology, and science at the nanoscale, typically dealing with particles smaller than 100 nm. It involves manipulating individual atoms and molecules to create nanomaterials with exceptional properties distinct from those of bulk materials. Nanotechnology has garnered extensive research interest due to its potential benefits across various scientific fields, including material science, biology, chemistry, physics, and engineering. Nanotechnology and nanomaterials have proven to be extremely beneficial and are now used in a variety of sectors, including biomedicine [1], biosciences, electronics, environmental protection, and optics. These materials have distinct chemical and physical properties, which provide substantial advantages over typical materials. Nanotechnology alters bulk materials, making them more efficient and beneficial. Because of its transformational potential, nanotechnology is currently a top priority for scientists. However, there is still much to find, as there is plenty of room at the bottom.

The performance of nanomaterials is significantly influenced by their dimensions or forms, as evidenced by their advanced functional application. For example, nanomaterials can take various forms, such as nanowires, nanorods [2], nanotubes [3], nanospheres [4], nano leaves [5], hierarchical nanostructures, nanoribbons [6], nanoshells, nanoplates, nanocages [7], nanoflowers [8], nanobuds, nano chains, nanosheets [3], nanorings [9], and nanoparticles [10]. In recent years, two-dimensional nanosheets of monoelemental materials such as phosphorene, silicene, antimonene, borophene, arsenene, germanene, plumbene, iodinene, and stanene have been extensively studied. This variety highlights the emphasis on the geometry and structure of nanomaterials rather than merely their size to enhance performance across different applications. In broader terms, these nanomaterials can be classified based on their dimensions. Materials that are nanostructured in zero dimensions (0D), one dimension (1D), two dimensions (2D), and three dimensions (3D). More focus has been placed on designing and organizing nanomaterials to satisfy the requirements of materials in various disciplines, including energy production, conversion, storage, and wastewater treatment. Nanomaterials are classified based on their nanoscopic dimensions.

Zero-dimensional (0D) nanomaterials have all three dimensions within the nanoscale, forming a nearly spherical shape. These materials are essentially point-like with no dimensions extending beyond the nanoscale—examples include quantum dots, nanoparticles, and nanoclusters.

One-dimensional (1D) nanomaterials have two dimensions confined to the nanoscale, with the third dimension extended. This results in a needle-like shape, often called nanowires, nanotubes, or nanorods—examples include carbon nanotubes (CNTs), nanowires, and nanoribbons.

Two-dimensional (2D) nanomaterials have only one dimension in the nanoscale, resulting in ultra-thin sheets or layers. They are often one or a few atoms thick and can be flexible or stackable. For examples graphene, transition metal dichalcogenides (like MoS_2), and hexagonal boron nitride (h-BN).

Bulk materials have no dimensions at the nanoscale; hence, they are considered bulk materials rather than nanomaterials. This chapter explores various types of 2D nanomaterials, detailing their synthesis methods, functional properties, and applications. It reviews recent advancements and showcases their significant potential.

TYPE OF 2D NANOMATERIALS

2D nanomaterials have emerged as a fascinating class with promising properties, and the discovery of graphene, a 2D atomically thin carbon sheet isolated from graphite in 2004, sparked significant interest in 2D nanomaterials. This breakthrough demonstrated that materials just one or a few atoms thick could achieve outstanding performance in various applications. Thus, the search for 2D nanomaterials intensified, leading to the discovery of numerous new 2D materials, both experimentally and conceptually. Significantly, notable progress has been achieved in the discovery and development of elemental 2D layered materials over the past few years, as illustrated in (Fig. **1**).

After graphene, the first 2D nanomaterial from the MXene family, Ti_3C_2Tx, was discovered at Drexel University in 2011 [12]. Silicene was introduced in 2012 as the first post-graphene substance. Subsequent discoveries include 2D materials like germanene, stanene, and plumbene. Extensive research has led to the discovery of a wide range of 2D nanomaterials. Examples include Layered Double Hydroxides (LDHs), silicate clays, Transition Metal Dichalcogenides (TMDs) like $NbSe_2$, MoS_2, $MoSe_2$, TaS_2, WS_2, and WSe_2, as well as transition metal oxides (TMOs), boron nanosheets (BNSs), graphitic carbon nitride (g-C_3N_4), black phosphorus (BP), antimonene (AM), hexagonal boron nitride (h-BN), and tin telluride nanosheets (SnTe NSs) [12]. These materials share structural features and exhibit various unique properties (Fig. **2**).

CHAPTER 2

Fundamentals of Supercapacitors

Vikas Kumar Pandey[1] and **Bhawna Verma**[1,*]

[1] *Department of Chemical Engineering and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi – 221005, India*

Abstract: This chapter thoroughly introduces the basics of supercapacitors, highlighting their critical role in contemporary energy storage solutions. The growing energy demand, driven by rapid technological advancements, has pushed the exploration of high-performance energy storage devices to new heights. The two primary energy storage devices, capacitors or electrochemical capacitors, supercapacitors, and batteries, stand out for their ability to store and supply energy from sustainable sources. Supercapacitors are particularly valued for their high power density and exceptional cycle stability. Supercapacitors provide a higher specific power density compared to lithium-ion batteries and fuel cells while offering greater energy density than traditional capacitors. In all these devices, energy transfer occurs at the interface between the electrode and electrolyte. For conventional capacitors, a dielectric material is positioned between two charged electrodes. A separator is used between the electrodes and the electrolyte solution in supercapacitors, fuel cells, and batteries. Overall, this chapter provides a foundational understanding of supercapacitors, presenting insights into both current progress and future trends in energy storage technology.

Keywords: Energy storage, Electric double-layer capacitors, Hybrid supercapacitors, Pseudocapacitors.

INTRODUCTION

The widespread reliance on fossil fuels, including oil, gas, and coal, has been vital in driving social and economic progress since the Industrial Revolution. However, the depletion of natural resources and their uneven distribution have created economic difficulties, including price volatility and supply chain disruptions, which negatively affect various sectors like energy production, industrial processes, and transportation [1 - 3]. Additionally, the widespread reliance on fossil fuels has led to significant carbon accumulation in the environment. With the growing demand for energy, the dependence on non-renewable resources continues to rise, contributing to increased pollution and greenhouse gas

* **Corresponding author Bhawna Verma:** Department of Chemical Engineering and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi – 221005, India; E-mail: bverma.che@itbhu.ac.in

Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma (Eds.)

emissions. Despite advancements in science and technology, the global energy demand persists, while the reserves of fossil fuels are steadily being exhausted [4 - 6]. The negative environmental effects of fossil fuel pollution, such as climate change and disruptions to ecosystems, have led to initiatives focused on adopting renewable energy sources like solar, wind, biomass, tidal, hydro, and geothermal energy. These renewable sources are considered sustainable and environmentally friendly, offering significant potential to replace fossil fuels. However, one key challenge is the intermittent nature of renewable energy, as production often depends on variable factors like weather. For instance, solar and wind energy output fluctuates based on sunlight and wind availability. This variability makes it difficult to ensure a steady energy supply. Energy storage systems are essential in tackling this challenge. They capture excess energy generated during peak production times and release it when required, maintaining a stable and reliable energy supply [7 - 9]. By improving the reliability of renewable energy, such systems can facilitate a shift to low-emission or zero-emission technologies, such as electric vehicles, and support the widespread adoption of renewable energy in homes, businesses, and industries [10, 11].

Energy storage is essential for maintaining the stability and reliability of modern energy systems. At present, significant amounts of energy are stored in hydrocarbons, including coal, oil, and natural gas, in both their raw and processed forms. This method is more efficient than storing electricity directly, as energy demand and generation fluctuate. An exception to this is pumped hydroelectric storage, which can rapidly increase energy output when needed. As energy systems increasingly adopt low-carbon technologies, the role and methods of energy storage are expected to evolve significantly. Two major trends are likely to drive these changes. Balancing electricity supply and demand is becoming increasingly difficult due to the variable nature of renewable energy sources and the constant output of nuclear power, which may result in potential mismatches. Unlike hydrocarbons, most low-carbon energy sources cannot be easily stored, with the exception of flexible gas generation, highlighting the need for advanced energy storage solutions in a future with reduced dependence on fossil fuels.

The shift to low-carbon energy sources for transportation and heating is expected to significantly alter electricity demand patterns. To manage this change, energy storage systems are developed to capture excess electricity during times of high production, making it accessible during peak demand. Additionally, these systems can transform surplus electricity into heat or hydrogen, enabling its use in various industries and expanding its role within the energy sector. Energy storage technologies will play a transformative role in advancing a low-carbon society. For example, condenser energy, which is considered low-quality energy, has a voltage output that varies based on its discharge state, unlike batteries that provide more stable energy output. Fuel cells, which rely on liquid fuels like methanol, can store substantial energy but typically deliver low power output. Meanwhile, lithium-oxygen batteries offer both low power and high energy density, making them highly efficient for certain applications. As these storage technologies continue to evolve, they will be critical in supporting the transition to a sustainable, low-carbon energy system.

The Ragone plot, as shown in Fig. (**1**), demonstrates the relationship between specific energy density and specific power density across various types of storage and conversion devices. The fuel cells have been shown to exhibit the highest specific energy density, meaning they can store a substantial amount of energy relative to their mass. However, their particular power density is lower, indicating a slower rate of energy delivery compared to devices like lithium-ion batteries, capacitors, and supercapacitors.

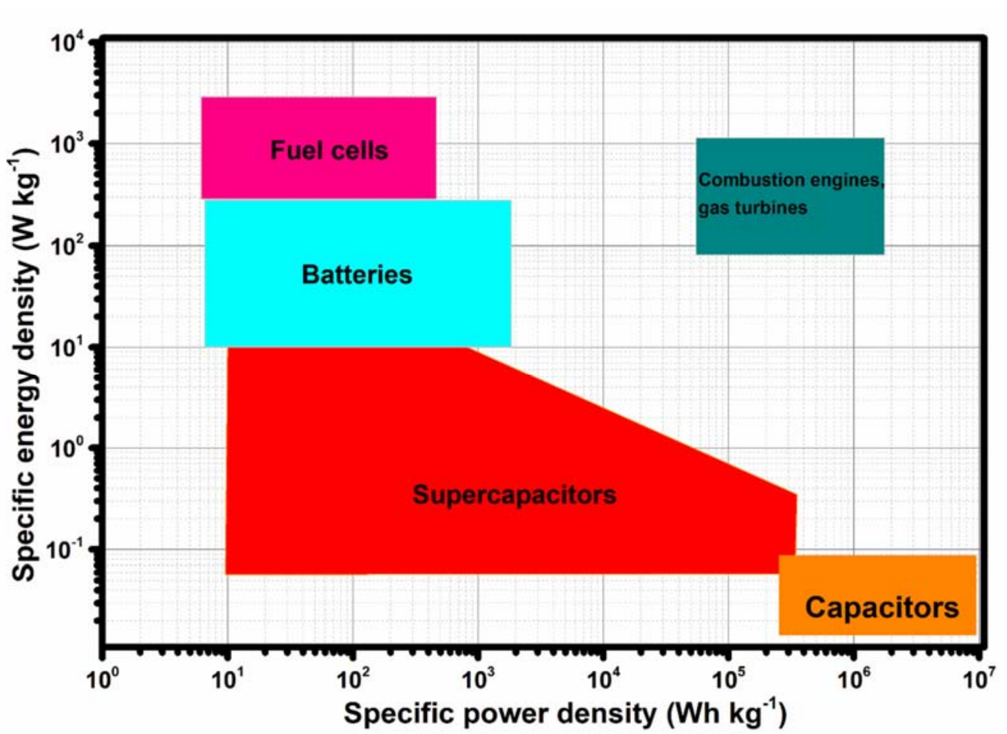

Fig. (1). Ragone plots for various energy storage and conversion devices.

CHAPTER 3

Graphene-based Functional 2D Nanomaterials for Energy Storage

Abhishek Kumar[1,*], **Hara Mohan Jena**[1] and **Krunal M. Gangawane**[2]

[1] *Department of Chemical Engineering, National Institute of Technology Rourkela, Rourkela-769008, Odisha, India*

[2] *Department of Chemical Engineering, Indian Institute of Technology Jodhpur, Jodhpur-342030, Rajasthan, India*

Abstract: Graphene-based two-dimensional nanomaterials have significant potential for energy storage because of their exceptional electrical conductivity (>10^6 S/m), mechanical strength (130 GPa), and vast specific surface area (2,630 m^2/g). These attributes enhance energy storage efficacy by augmenting energy densities, cycle stability, and ion movement. Doping with heteroatoms and incorporation with transition metal oxides have shown potential. Graphene-based anodes may exceed the performance of conventional graphite anodes (372 mAh g^{-1}) with capacities reaching 900 mAh g^{-1}. Hybrid materials consisting of graphene and MnO_2 demonstrate an energy density of 150 Wh/kg, a specific capacity of 1,494 mAh g^{-1}, and remarkable cycle stability. Elevated production costs (exceeding $100 per gram for premium graphene) and the ecological impact of high-temperature synthesis methods (surpassing 1,000°C) persist as challenges. Future research should prioritise scalable and cost-effective manufacturing, advanced functionalisation for material properties, and artificial intelligence to enhance synthesis and device performance. Several obstacles must be addressed to optimise graphene-based energy storage technologies.

Keywords: 2D-nanomaterials, Energy storage, Graphene, Lithium-ion batteries (LiBs), Nanocomposites, Supercapacitors.

INTRODUCTION

In 2024, the world population exceeded 8 billion, and rapid technological advancements have significantly increased the demand for energy, resulting in a remarkable 60% rise in global energy consumption over the last 30 years. Fossil fuels, now constituting around 80% of worldwide energy output, are limited and have significant environmental repercussions, including the emission of almost 33

* **Corresponding author Abhishek Kumar:** National Institute of Technology Rourkela, Rourkela-769008, Odisha, India; E-mail: abhisheknitrkl@outlook.com

Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma (Eds.)

billion metric tonnes of CO_2 per year, which contributes to the acceleration of climate change and global warming. Researchers are currently seeking techniques to diminish or eliminate dependence on fossil fuels to address these issues [1 - 3].

Strategies to reduce reliance on fossil fuels concentrate on three primary approaches. Initially, improving energy efficiency in traditional systems, such as by waste heat recovery, may recover up to 30% of energy used during industrial operations. Secondly, sustainable energy conversion technologies such as proton-exchange membrane fuel cells, which have efficiencies of over 60%, provide environmentally benign alternatives to conventional energy systems. Third, renewable energy sources such as solar, wind, biomass, and ocean sustainably fulfil global energy requirements [4]. Solar energy has a yearly potential of 1,575 and 49,837 exajoules (EJ), far surpassing world power consumption, but wind energy is predicted to provide around 117GW in 2023 annually [5]. The usage of renewable energy has increased markedly, with extensive initiatives showcasing its feasibility. The Three Gorges Dam in China, the most extensive hydroelectric power facility, has an installed capacity of 22,500 MW, generating 87 TWh of energy each year, sufficient to power roughly 80 million households [6]. The Gansu Wind Farm, with a capacity of 7,965 MW, produces around 20 TWh per year [7]. The irregularity of renewable energy continues to pose a significant problem. Additionally, solar power plant capacity may be restricted by up to 70% on overcast days, while wind turbine production may be reduced by as much as 100% on calm days [8 - 10].

Such variability underscores the urgent need for robust energy storage systems to bridge supply and demand gaps effectively. Consequently, the global energy storage market is expected to experience significant growth, increasing from 20 GW in 2022 to a projected 500 GW by 2030, primarily driven by the integration of renewable energy sources [11]. Among current technologies, lithium-ion batteries (LiBs) dominate the market due to their high energy densities of 250–300 Wh/kg, coupled with their efficiency and reliability [12]. Despite these advantages, the scalability of LiBs is constrained by high costs and reliance on limited resources, such as lithium and cobalt. These challenges highlight the critical need for the development of more advanced, efficient, and sustainable energy storage alternatives to support the expanding renewable energy landscape. 2D nanomaterials, particularly graphene and its derivatives, are transformational energy storage materials due to their exceptional electrical and structural characteristics [13 - 16].

Graphene, a hexagonal carbon monolayer, has unusual electrical conductivity (>10^6 S/m), tensile strength (130 GPa), and specific surface area (2,630 m^2/g). It improves energy density, power output, and stability in energy storage technologies, including supercapacitors, batteries, and hybrid systems. For supercapacitors that store and release energy quickly, the high electrical conductivity of graphene expedites electron transport and charge and discharge cycles. The energy density of graphene-based supercapacitors may reach 85 Wh/kg, exceeding standard supercapacitors while maintaining excellent power output and cycle life. Composite materials or hybrid systems integrate unique properties of graphene with complementary nanomaterials to maximise performance. Its energy storage flexibility is enhanced by graphene oxide (GO), reduced graphene oxide (rGO), and graphene-based composites. Functional groups on GO make chemical modifications and integration with polymers, metals, and metal oxides easier, improving energy storage and material durability. However, rGO, which preserves most of the graphene's conductivity, is cheaper for practical applications. Hybrid architectures using graphene, transition metal oxides, conducting polymers, and carbon nanotubes provide energy densities of up to 200 Wh/kg, high power density, and excellent cycle stability. Graphene anodes improve energy density and cycle life in battery technology. LiBs with graphene anodes might improve charge capacity by 50% relative to graphite anodes. The remarkable thermal conductivity of graphene facilitates efficient heat management when charging and discharging, mitigating the risk of thermal runaway and extending battery lifespan [17 - 20].

Function of revolutionary graphene supercapacitors. These devices can rapidly charge and discharge, enduring over 1,000,000 cycles, making them appropriate for electric car regenerative braking and uninterruptible power sources. Graphene supercapacitors charge more rapidly than LiBs, achieving full charge in minutes. Nevertheless, with these benefits, the mass production of high-quality graphene at an economical price remains challenging. The research seeks to create scalable and economical synthesis techniques that maintain the material's intrinsic features. Consistent distribution, material stability, and compatibility with other storage components are essential for the integration of graphene into commercial energy storage systems. The chapter analyses graphene-based 2D nanomaterials for advanced energy storage applications by examining their properties, integration strategies, and performance enhancement methods while addressing scalability and production challenges [21 - 24].

GRAPHENE AND ITS DERIVATIVES

Graphene, a material with remarkable properties, is a monolayer of sp^2-hybridized carbon atoms arrayed in a hexagonal lattice. This is possible due to the unique atomic structure of graphene. Graphene most extensively interacts with molecules, ions, and nanoparticles among known materials, as evidenced by its theoretical surface area of 2630 m^2/g. Subsequently, it is an optimal material for

CHAPTER 4

MXene-based Functional 2D Nanostructures for Energy Application

Pallab Bhattacharya[1,2,*], **Arnab Samanta Roy Choudhury**[1] and **Abhinaba Das**[1]

[1] *Functional Materials Group, Advanced Materials & Corrosion (AMC) Division, CSIR-National Metallurgical Laboratory (NML), Burmamines, East Singhbhum, Jamshedpur, Jharkhand - 831007, India*

[2] *Academy of Scientific & Innovative Research (AcSIR), Ghaziabad - 201002, India*

Abstract: MXenes, a rapidly emerging class of two-dimensional (2D) materials composed of transition metal carbides, nitrides, and carbonitrides, have gained significant attention for their exceptional properties, such as high electrical conductivity, hydrophilicity, tunable surface chemistry, and large specific surface area. Interestingly, the functionalisation of MXenes and optimized tuning of their functional properties can play a very important role in controlling a wide range of energy applications, including energy storage, generation and conversion. Therefore, this chapter, specifically, delves into the design and development of MXene-based functional 2D nanostructures tailored for energy applications. Briefly, this chapter explores the strategies involved for fabricating various MXene-based functional 2D nanostructures, emphasizing their properties and role in improving energy storage, conversion, and generation capability. Furthermore, the integration of MXenes with other nanomaterials to create multifunctional composites and their potential to address current challenges in energy technologies has also been addressed. By highlighting the progress and potential of MXene-based nanostructures, this chapter aims to provide a comprehensive overview of their use in innovative energy devices and offers insights into future research directions to harness their full potential for sustainable and efficient energy solutions.

Keywords: 2D nanostructures, Energy generation, Energy storage, Functionalization, MXene.

INTRODUCTION

As the demand for sustainable energy keeps growing, there is an increasing focus on developing materials that can make energy generation, storage, and conversion

* **Corresponding author Pallab Bhattacharya:** Functional Materials Group, Advanced Materials & Corrosion (AMC) Division, CSIR-National Metallurgical Laboratory (NML), Burmamines, East Singhbhum, Jamshedpur, Jharkhand - 831007, India; E-mail: pallab.nml@csir.res.in

Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma (Eds.)

and storage more efficient. In electrochemical energy applications, a material's surface area, morphology, and redox properties play a big role, helping with processes like ion movement, adsorption, and chemical reactions [1]. This is where 2D materials like graphene [2], borophene [3], phosphorene [4], transition metal dichalcogenides [5], and MXene [6] stand out as they have huge surface areas and high electrical conductivity, making them well-suited for various energy applications [7, 8].

For applications like Supercapacitors (SCs), batteries, and water-splitting catalysts, 2D materials have some great advantages due to their crystalline structure which makes it easy for electrons to move quickly, their layered structure which provides plenty of paths for ions to flow through, and the 2D form helps manage volume changes during reactions while keeping a solid connection between nanosheets [2, 4]. This unique combination of properties makes them powerful tools in modern energy solution technologies. Since the discovery of Ti_3C_2 in 2011 [9], 2D materials known as MXene, comprising transition metal carbides, nitrides, and carbonitrides, have been rapidly gaining attention. Often referred to as rising stars, MXenes are celebrated for their remarkable similarity to graphene. One reason for this comparison is that both graphene and MXenes can be made using a top-down exfoliation technique, where the bulk material (graphite for graphene or a MAX phase for MXenes) is carefully thinned down to just one or a few atomic layers [10]. This method allows for the large-scale production of ultra-thin, 2D materials that exhibit unique properties because of their thickness. Moreover, MXenes are also known for their excellent metallic conductivity and abundant redox active sites, making them a promising candidate for various energy applications [10, 11].

Although MXenes have excellent electrical, chemical, and physical properties, they come with a few challenges. Over time, they can lose chemical stability as they are prone to oxidation and they also have a tendency to stack together, which reduces their surface area and limits their effectiveness [12]. To address these issues, scientists have recently been focusing on synthesizing MXene-based 2D nanostructures that improve stability and help MXenes reach their full potential in energy generation, storage, and conversion technologies. These nanostructures bring important advantages over bare MXenes and other 2D materials. They offer more customizable surfaces, better spacing between layers, and stronger structural stability. With these enhancements, nanostructured MXenes allow for faster ion movement, making them particularly effective for energy storage applications [12, 13, 6].

This chapter provides an in-depth analysis of MXene-based functional 2D nanostructures, with a particular focus on their synthesis, structural and electronic properties, and their applications in energy generation, storage, and conversion technologies. It examines the various synthesis techniques used to develop various MXene-based 2D nanostructures, as well as the unique properties that make them ideal for energy-related applications, such as high conductivity and large surface area. The chapter also addresses the current challenges in MXene synthesis, including issues related to stability, scalability, and performance degradation. Potential solutions and strategies for overcoming these challenges are discussed, along with insights into the future development of MXenes. Ultimately, this chapter highlights the transformative potential of MXenes in advancing sustainable energy technologies, offering a forward-looking perspective on their role in addressing global energy demands and contributing to a greener future.

PREPARATION, STRUCTURE, AND PROPERTIES OF MXENE

This section discusses various conventional and non-conventional synthesis methods of MXenes and their influence on quality and composition. It also explores their layered structure, tunable interlayer spacing, and surface functional groups, which affect their electrochemical and chemical stability. Finally, it highlights MXenes' exceptional electrical, magnetic, optical, and mechanical properties, making them ideal for energy applications like SCs, batteries, catalysis, sensors, and Electromagnetic interference shielding (EMI).

Preparation of MXenes

MXenes can be synthesized by selective etching the A layer from MAX phases, using fluoride-based as well as fluoride-free etching techniques. In this subsection, we have highlighted various etching methods and their advantages and disadvantages.

Etching with Fluorine-Containing Acids

Fluorine-based etching, commonly using hydrofluoric acid (HF), is a conventional method for synthesizing MXenes developed by Gogotsi *et al.* in 2011 [9], and remains the most effective when it comes to the synthesis of $Ti_3C_2T_X$ MXene. The etching reactions are detailed as follows [9]:

$$Ti_3AlC_2 + 3HF \rightarrow AlF_3 + 3/2H_2 + Ti_3C_2 \quad \textbf{(1)}$$

$$Ti_3C_2 + 2H_2O \rightarrow Ti_3C_2(OH)_2 + H_2 \quad \textbf{(2)}$$

$$Ti_3C_2 + 2HF \rightarrow Ti_3C_2F_2 + H_2 \quad \textbf{(3)}$$

CHAPTER 5

Application of 2D-MOF Materials in Energy Storage

Vishwa Pratap Singh[1,*], **Satyendra Kumar Satyarthi**[2] and **Chandra Bhal Singh**[2]

[1] *UNAM - National Nanotechnology Research Center and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara - 06800, Türkiye*

[2] *School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi-221005, India*

Abstract: Metal-organic Frameworks (MOFs), characterized by their high surface area, adjustable pore dimensions, structural diversity, and a wide array of periodic organic-inorganic components, have emerged as highly adaptable precursors or templates for developing functional materials. These materials find significant use in advanced electrodes or catalysts that facilitate efficient electrochemical energy storage (EE). This chapter outlines various strategies for designing these materials, demonstrating the extensive range of possible chemical compositions and physical structures derived from MOFs, then emphasizes recent developments, particularly focusing on the relationships between composition, structure, and performance, and explores their practical applications across different EE systems, including supercapacitors, rechargeable batteries. The chapter concludes with a discussion on potential solutions for MOF-derived functional materials in EE, aiming to provide guidance for the future progress of this dynamic research area.

Keywords: 2D Materials, Batteries, Energy storage, MOF, Supercapacitors.

INTRODUCTION

With rapid advancements in global economies and societies, the past decade has seen a notable improvement in living standards. However, this progress has been accompanied by environmental challenges, including increased emissions of CO_2, SO_2, CH_4, N_2O, and other harmful gases. These pollutants contribute to global warming and ecological degradation, posing significant threats to sustainable development. To mitigate these pressing issues, a transition to renewable energy

* **Corresponding author Vishwa Pratap Singh:** UNAM - National Nanotechnology Research Center and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara - 06800, Türkiye;
E-mail: vishwasodan@gmail.com

Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma (Eds.)

source-such as solar, wind, and tidal power-has gained substantial momentum. The inherent variability of renewable energy sources poses a significant hurdle to their large-scale adoption. To address this challenge, the development of cutting-edge energy storage solutions, such as advanced batteries and supercapacitors, has become crucial in synchronizing energy supply and demand. Existing energy storage technologies, however, face limitations. Batteries are often constrained by low power density, while supercapacitors struggle with limited energy density. Novel electrode materials are urgently needed to boost energy storage efficiency and scalability. Metal-organic Frameworks (MOFs) offer a promising solution, leveraging their exceptional structural and chemical properties [1 - 3]. MOFs are highly ordered crystalline materials characterized by a unique architecture where metal ions or clusters act as nodes, and organic molecules, known as linkers or ligands, form bridges between these nodes. These frameworks are held together by strong coordination bonds, which provide stability and define their intricate porous structures. Their distinctive porous structure, adaptable architecture, thermal stability, and vast surface area render them exceptionally versatile for diverse applications. These applications include catalysis, gas storage, sensing, separation, and energy storage. The flexibility of MOFs is further amplified by the ability to tailor their properties through deliberate variations in metal cations, organic linkers, and synthesis methods. This customization capability enables researchers to design MOFs with specific properties, making them suitable for a wide range of uses. Since the pioneering synthesis of the first MOF material—layered cobalt-homophthalic acid—in 1995, the field has witnessed explosive growth, with over 20,000 MOFs documented by 2022. This remarkable progress underscores the vast potential of MOFs and their likely impact on various industries and applications [4, 5].

The intrinsic attributes of MOFs, such as their customizable framework and high density of active sites, offer significant advantages for electrochemical energy storage. Their porosity allows for efficient ion diffusion, while the tunability of their chemical composition provides opportunities to optimize their redox activity. However, traditional three-dimensional (3D) MOFs face several challenges that limit their performance in energy storage devices. These include sensitivity to moisture, which can degrade their structure and reduce their surface area, and poor electrical conductivity, which hampers their rate performance [6, 7]. Additionally, the narrow micropores of many 3D MOFs restrict rapid ion diffusion, and the incomplete exposure of active sites reduces their interaction with ions, thereby limiting their electrochemical capacity. To address these shortcomings, scientists have concentrated on refining the internal framework and electrical properties of MOFs, while also streamlining their architectural configuration. Advances in synthesis techniques have enabled the development of two-dimensional 2D- MOFs, which exhibit enhanced properties compared to their

3D counterparts [8, 9]. The 2004 discovery of graphene sparked intense interest in 2D materials, leading to the emergence of novel 2D-MOFs, transition metal disulfides, black phosphorus, and noble metal nanomaterials. Characterized by ultra-thin layers of atoms or molecules, these 2D materials exhibit robust intra-layer bonding and weak inter-layer interactions. This distinctive configuration imparts remarkable attributes, including enhanced electrical conductivity, expansive interfacial regions, and accelerated electron mobility. The integration of 2D structures with MOFs has been particularly effective in improving their performance in energy storage applications [10, 11]. As compared to 3D MOFs, 2D-MOFs feature exposed active sites, facilitating deep interactions with electrolyte ions. Their high aspect ratio, layered structure, and large surface area enhance anisotropic properties, improve ion storage, and mitigate structural aggregation during electrochemical cycling. Additionally, their layered architecture effectively accommodates mechanical stress, reducing volume changes and enhancing electrode stability during charge-discharge processes [12, 13]. The conductivity can be enhanced for the 2D-MOFs. As a result, 2D-MOFs have shown remarkable electrochemical performance in recent studies [14, 15]. Despite their potential, research on 2D-MOFs in energy storage is limited, but combining them with other advanced materials holds promise for overcoming existing limitations. Leveraging 2D-MOFs' unique characteristics, researchers aim to develop next-generation electrode materials with high energy density, power density, and cycling stability [16, 17].

This chapter provides a comprehensive review of 2D-MOF-based electrode materials for energy storage, highlighting recent advances in synthesis, design, and performance. Through a detailed exploration of 2D-MOFs and their composites, this discussion aims to shed light on the potential of these materials to revolutionize energy storage technologies and support the transition toward sustainable energy solutions.

MOFS FOR BATTERY ENERGY STORAGE

Traditional cathode materials in Lithium-ion Batteries (LIBs), such as $LiCoO_2$ [18] and $LiFePO_4$ [19], have limited capacity and compromised rate performance. Alternative materials, including $LiMn_XO_X$ [20], $LiNiO_2$ [21], and $LiNi_XCo_XMn_XO_2$ [22], have been explored, but their capacities are difficult to improve beyond 300 mAh/g. The unique pore structure of MOFs makes them suitable for lithium storage and ion transmission, leading to recent research focusing on developing MOFs for high-energy and power-density cathode materials [23].

CHAPTER 6

Covalent Organic Framework-Based Functional 2D Materials for Energy Applications

Vidhya K.V.[1] and **Simi Pushpan K.**[1,*]

[1] *Department of Chemistry, Union Christian College, Aluva, Kerala - 683102, India*

Abstract: Covalent Organic Frameworks (COFs) are the newest and fast-growing field of microporous crystalline polymers with 2D and 3D frameworks that emerged after the development of reticular chemistry. 2D COF nanosheets possess unique properties such as large surface area, ultrathin thickness, and high porosity, along with flexibility in design and synthesis, tunable structure, and chemical modification, which make them versatile enough to be utilized for gas separation and storage, sensing, catalysis, energy conversion, optoelectronics and drug administration. The distinctive morphological design features of 2D COFs perfectly position them for energy applications involving supercapacitors, metal-ion batteries, photocatalysis, and electrocatalysis. The highly ordered π–π stacked orientation of 2D COFs provides pathways for the efficient transport of charge carriers like ions, electrons, and holes through the conjugate skeleton. 2D COFs, owing to their adjustable pore sizes, can efficiently capture and release mobile ions of varying sizes and charges in the nanosheets, and the functionalization of the pore system with redox-active species enhances its redox capabilities. The covalently linked framework and non-metallic nature of COFs provide exceptional scaffold stability and reversibility, enabling a prolonged life cycle. This book chapter provides an insightful review of recent developments in the 2D COF field with an emphasis on molecular design, synthetic methods, and energy-related applications.

Keywords: Covalent Organic Frameworks (COFs), Energy applications, Multifunctional materials, Rechargeable metal-ion batteries, Supercapacitors.

INTRODUCTION

Covalent Organic Frameworks (COFs) belong to a newly emerging group of microporous crystalline solids characterized by distinct 2D or 3D frameworks [1, 2]. COFs are the second primary outcome of reticular chemistry, promoting the controlled synthesis of highly organized, porous crystalline structures. Owing to their outstanding features, COFs quickly grabbed the scientific community's

* **Corresponding author Simi Pushpan K.:** Department of Chemistry, Union Christian College, Aluva, Kerala - 683102, India; E-mail: simi.pushpan@uccollege.edu.in

Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma (Eds.)

attention and established themselves as a formidable rival to similar framework structures. COFs can be synthesized by combining organic monomers with strong covalent linkages, resulting in stiff, low-density, highly resistant, and stable structures. The geometry of these building blocks dictates the crystalline framework, exhibiting regular patterns and diverse pore sizes [3].

Among the various types of COFs, highly oriented COF nanosheets, also known as 2D COFs, have garnered considerable interest among researchers as an organic material holding enormous promise owing to their multifaceted characteristics. 2D-COFs consist of layered structures formed by stacking $\pi-\pi$ interactions. Within each layer, covalent bonds provide structural integrity while non-covalent interactions improve stability, thereby contributing to the overall functionalities of these materials. Interactions of 2D COFs with various elements such as electrons, holes, ions and molecules can be tuned by altering pore and skeletal design [5]. 2D COFs, with their uniform porous structure, high crystallinity, large specific surface area, transformable structure, low density and high thermal/chemical stability, are being investigated for catalytic, sensing, and storage applications (Fig. **1**). Desired 2D COFs with specific structures and properties can be designed and synthesized using variety of precursors which allows us to control its physical, optical and electrical properties thereby expanding the scope of their applications [6, 7].

Multifunctional COFs are widely explored as a sustainable option in the energy field, particularly for rechargeable batteries and supercapacitors. COFs have distinct advantages, including highly cross-linked structure, porosity and pi-conjugation, making them ideal electrode materials. In battery applications, COFs serve multiple purposes as electrode materials, such as storing energy, transporting ions, host materials and blocked layers. The issue of increasing battery volume is mitigated by the extensive specific surface area of COFs due to their high porosity. AA stacking patterns in COFs create one-dimensional channels that allow them to function as charge transporters and host materials. AB stacked COFs, which lack channels and have a closely packed network structure, hinder molecular transport and safeguard electrodes [8]. A newly reported benzimidazole-linked COF (BCOF-1) exhibiting a high theoretical specific capacity value demonstrates the advancement of redox-active COFs in sodium ion storage for efficient batteries. It crystallizes with an eclipsed AA stacking forming hexagonally shaped mesoporous one-dimensional channels, characterized by a substantial surface area that promotes accelerated charge transfer and ionic mobility [9].

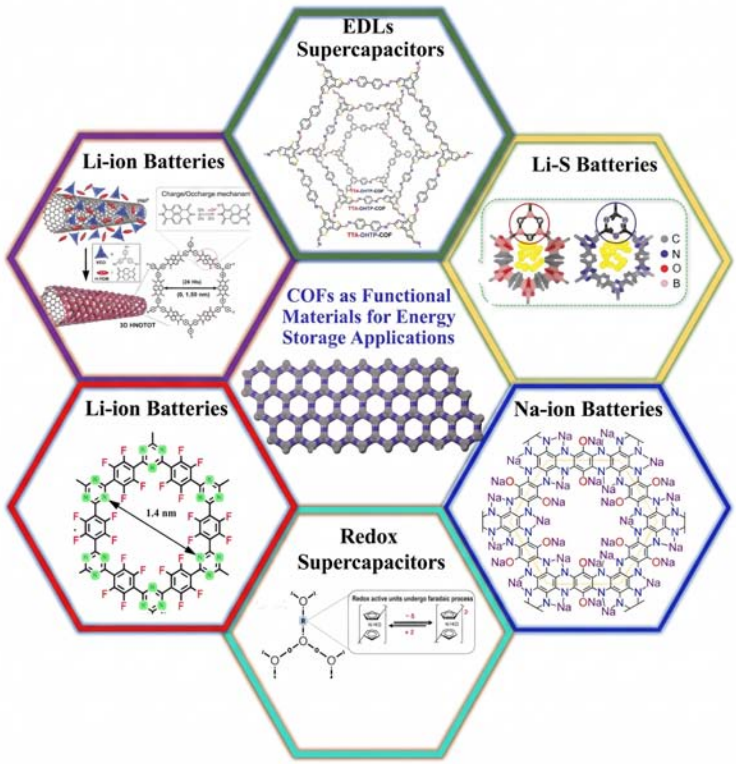

Fig. (1). General applications of 2D COFs [4].

MXene@COF composites are among the latest rapidly emerging multifunctional materials with a wide range of applications including energy (Fig. **2**). MXenes, the newest class of 2D layered transition metal compounds (*e.g.* $Ti_3C_2T_x$, V_2CT_x*etc.*), are known for their unique surface chemistry [10]. Its high conductivity made it employable in Lithium-sulphur batteries. The nonporous structure of MXenes imposes limitations, such as poor sulphur loading and an ineffective ion diffusion rate. However, when combined, COFs and 2D MXenes work together to improve their properties, resulting in a composite that has high electrical conductivity, chemical stability and porosity [11]. Moreover, the ability to tune both the structure and functionality further establishes them as a superior material for emerging technologies [12]. COF-2D MXene hybrids have been extensively explored for various energy applications, including batteries such as LIBs, LSBs, SIBs, and ZABs, as well as supercapacitors, showing outstanding performance because of the synergistic effects of hybridization [13].

CHAPTER 7

Transition Metal Oxide Based Functional Materials for Electrochemical Energy Storage

Shreeganesh Subraya Hegde[1,2,*], **Dibyananda Majhi**[1], **Badekai Ramachandra Bhat**[3] and **Challapalli Subrahmanyam**[1]

[1] *Energy and Environmental Laboratory, Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy 502285, Telangana, India*

[2] *Department of Chemistry, School of Engineering, Dayananda Sagar University, Harohalli, Bengaluru, Karnataka 562112, India*

[3] *Catalysis and Materials Chemistry Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, Mangalore 575025, Karnataka, India*

Abstract: Supercapacitors are emerging as a compelling energy storage solution, enhancing superior power density, extended charge-discharge cycles, and improved safety compared to traditional batteries. Developments in supercapacitor technology, especially in the innovative design and refinement of electrode materials, represent a substantial leap forward in addressing the world's growing energy storage needs. In the pursuit of advancing electrode materials, the study and utilization of 2D materials and their derivatives have revealed significant potential. These materials have emerged as highly promising candidates due to their mechanical strength, high surface area, and exceptional electrochemical properties. Among these, transition metal oxides stand out as a cutting-edge class of materials with highly favorable applications in supercapacitor electrodes. Their abundant resources and low production costs are significant advantages for large-scale supercapacitor production. This chapter offers an in-depth exploration of supercapacitor technology, emphasizing the latest breakthroughs in electrode materials and their effects on performance. It also underscores the pivotal role of transition metal oxides in realizing high-capacity and efficient energy storage systems. Finally, the chapter outlines the existing limitations and challenges associated with the development and use of transition metal oxides. It also delves into potential solutions and future directions, offering a comprehensive overview of the strategies needed to overcome these obstacles and advance the use of transition metal oxides in energy storage technologies.

Keywords: Clean energy, Electrode materials, Energy storage, Supercapacitor, Transition metal oxide.

* **Corresponding author Shreeganesh Subraya Hegde:** Energy and Environmental Laboratory, Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy 502285, Telangana, India;
E-mail: hegdeshreeganesh@gmail.com

Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma (Eds.)

INTRODUCTION

Climate change is now an alarming problem worldwide. The rapid heating of the Earth at an unprecedented rate significantly impacts the environment, leading to catastrophic climate changes [1, 2]. Currently, the burning of fossil fuels to meet global energy demands is a major contributor to the release of various greenhouse gases, which are responsible for this undesirable warming of the Earth [3]. Renewable green energy has become a key alternative to the aforementioned non-renewable fossil fuels [4]. Hydroelectric, tidal, solar, and wind energy are clean, renewable energy resources that emit little to no greenhouse gases. Generating green energy from the above resources is one of the most effective approaches to addressing the energy crisis without harming the earth's climate [5]. Although there has been a lot of research progress in these energy generation technologies, we cannot access them all the time in a day according to our needs without storing them because these energy productions depend on several factors, such as sunny weather or wind flow [6]. It is now imperative to develop an integrated approach for large-scale green energy generation coupled with efficient energy storage technologies for long-term use. This is evident from the intensive research efforts from the scientific community throughout the globe on sustainable storage technologies alongside energy conversion [5]. Various energy storage technologies have been developed for multiple purposes, including thermal energy storage, compressed air energy storage, pumped hydro storage, and electrochemical energy storage, such as capacitors, Supercapacitors (SC), and batteries [7].

Many recent developments and upgrades have been observed in the field of energy storage research to efficiently store energy converted from various renewable resources [8, 9]. Among all energy storage devices, batteries, including Li-ion, lead-acid, nickel-cadmium, and flow batteries, have widespread applications and dominate the energy storage technology market due to their high energy density [5]. Despite their widespread use, both rechargeable and non-rechargeable types of batteries exhibit several disadvantages. These include relatively low power density, which affects their ability to deliver high energy output in a compact form. Safety concerns also arise due to risks such as thermal runaway, leakage, or explosion, particularly with specific chemistries. Additionally, the heating effect during charge and discharge cycles can compromise battery performance and safety [10]. Environmental concerns are also significant, given the challenges related to the disposal and recycling of batteries, which often involve hazardous materials and contribute to environmental pollution [11]. Hence, batteries cannot alone solve the energy storage requirement with optimum efficiency [12]. On the other hand, Supercapacitors (SCs) offer distinct advantages in several aspects. For instance, SCs are superior to batteries in terms of power density (500 - 10,000 W/kg), lifespan (500,000 hours), wide operating temperature range, safety, and low internal resistance [13]. Unlike traditional batteries, which often have slower charge and discharge rates due to electrochemical reactions, supercapacitors leverage electrostatic interactions to store and release energy. This allows them to charge and discharge much more quickly [14]. In addition, SCs can be scaled up for use in both small electronic devices and large-scale applications with minimal environmental concerns. However, SCs exhibit a lower specific energy density compared to batteries, as clearly shown in the Ragone plot depicted in Fig. (**1**). Employing high-performing electrodes has been an intensive approach to enhancing the energy density of SCs [15]. The Ragone plot gives the idea that going from supercapacitors to hybrid systems, a high energy density and power density can be reached. Hence, significant research efforts are being put into the advancement of supercapacitors.

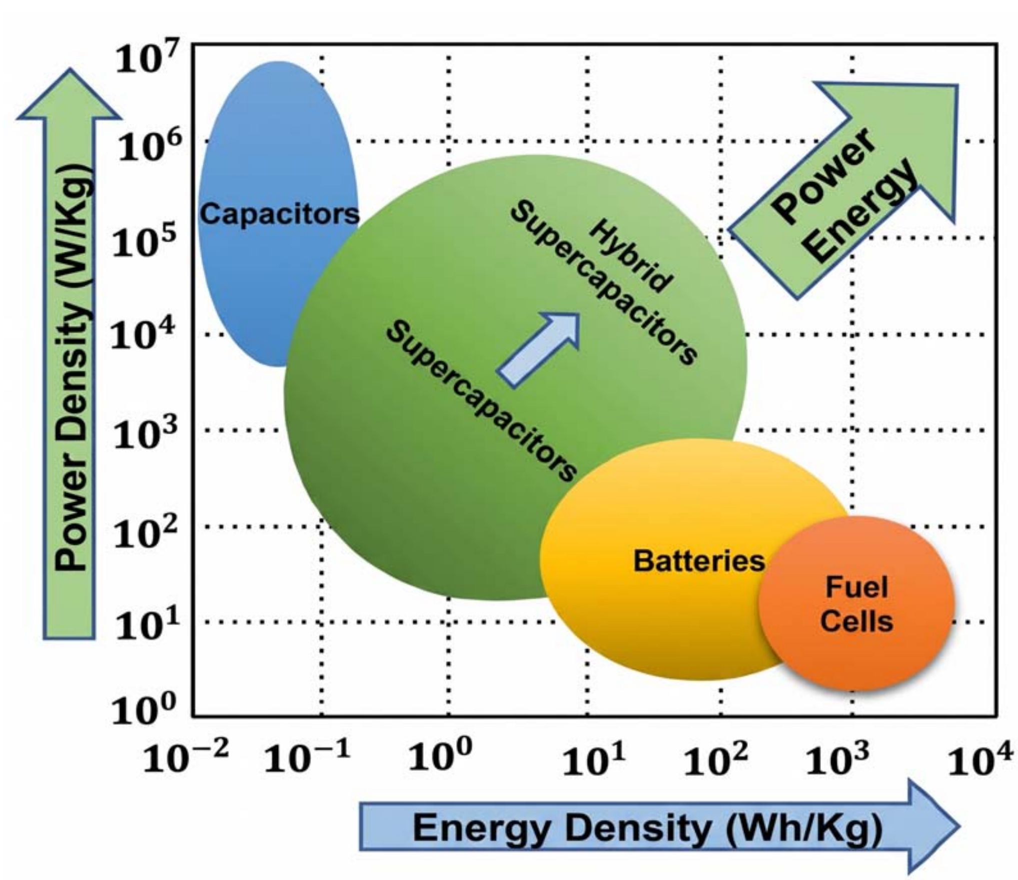

Fig. (1). A representative Ragone plot for different energy storage devices (adapted from [1]).

CHAPTER 8

Chalcogenides-based Functional 2D Nanostructure for Energy Storage Application

Dipsikha Ganguly[1,*], **Ponraj Jenis**[2], **Rayavarapu Prasada Rao**[1] and **Seeram Ramakrishna**[1]

[1] *Mechanical Engineering, National University of Singapore, Singapore*

[2] *Chemical and Biomolecular Engineering, National University of Singapore, Singapore*

Abstract: Two-dimensional (2D) chalcogenide materials have gained tremendous interest for energy storage applications because of their unique characteristics, such as high surface area, high conductivity, and many other chemical compositions. The focus of this chapter is the recent development of chalcogenide-based 2D nanostructures designed for a supercapacitor electrode. The chapter attempts to synthesize 2D chalcogenide materials with a desired architecture, composition, and defects through different synthesis methods, which include Chemical Vapor Deposition (CVD), hydrothermal/solvothermal methods, and exfoliation of layers. The assessment of those electroactive materials as the active components of supercapacitor devices is performed on the performance metrics of specific capacitance, energy density, power density, and cycling stability for different chemistries. Also, in this chapter, the improved performance of chalcogenide supercapacitors is discussed, such as the incorporation of dopants, composites with different materials, and the engineering of the structure of chalcogenides. The challenges and future directions of devices are also discussed. To summarize, this chapter highlights recent advances made in chalcogenide-based 2D nanostructures for supercapacitors in research and commercial applications.

Keywords: Chalcogenides, Energy storage, Supercapacitor, Two-dimensional.

INTRODUCTION

The global energy landscape is experiencing a marked increase in demand, driven by several critical factors such as population expansion, rapid urbanization, and economic growth. Projections suggest that by 2050, overall global energy requirements will rise by around 21%, with electricity consumption expected to almost double within the same timeframe [1, 2].

* **Corresponding author Dipsikha Ganguly:** Mechanical Engineering, National University of Singapore, Singapore; E-mail: dips11@nus.edu.sg

Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma (Eds.)

Key statistics highlighting this trend include:

- **Population Growth:** The world's population is anticipated to rise from approximately 8 billion in 2024 to nearly 9.8 billion by 2050, placing substantial pressure on energy systems to meet the increased demand.
- **Electricity Demand:** The need for electricity is growing at nearly twice the rate of overall energy consumption. This surge is largely attributed to the electrification of various sectors, such as transportation and industrial processes.
- **Dependence on Fossil Fuels:** Despite gradual progress towards adopting low-emission energy sources, fossil fuels remain a significant part of the global energy mix. In 2022, fossil fuels accounted for approximately 79% of the world's total primary energy supply. While this is projected to decline to 60% by 2050 under current policy frameworks, fossil fuels remain a significant part of the energy equation.

Supercapacitors, a type of energy storage system, have gained significant attention from industry experts in recent years [3]. In electrical systems, energy storage devices play a critical role by storing surplus energy during periods of high production and releasing it as needed. Bigger energy storage technologies, such as hydropower devices and compressed air energy storage, are commonly employed in power plants for bulk energy management. Conversely, batteries are well-suited for a broader range of medium- and short-term energy storage needs. These include distributing energy to remote locations, powering electric vehicles, supporting small-scale generation, off-grid storage for homes or buildings, and portable electronic devices.

In contrast to batteries, Supercapacitors (SCs) are high-power devices designed to deliver energy at rapid rates. They are primarily utilized in short-duration applications where quick bursts of electricity are required. Fig. (**1**) illustrates the Ragone plot, demonstrating the trade-off between energy density and power density for supercapacitors, batteries, and capacitors. Supercapacitors, often referred to as ultracapacitors, double-layer capacitors, or electrochemical capacitors, operate differently from conventional capacitors and batteries. While they may be conceptually described as a hybrid between a capacitor and a battery, their underlying principles and functions are distinct [4].

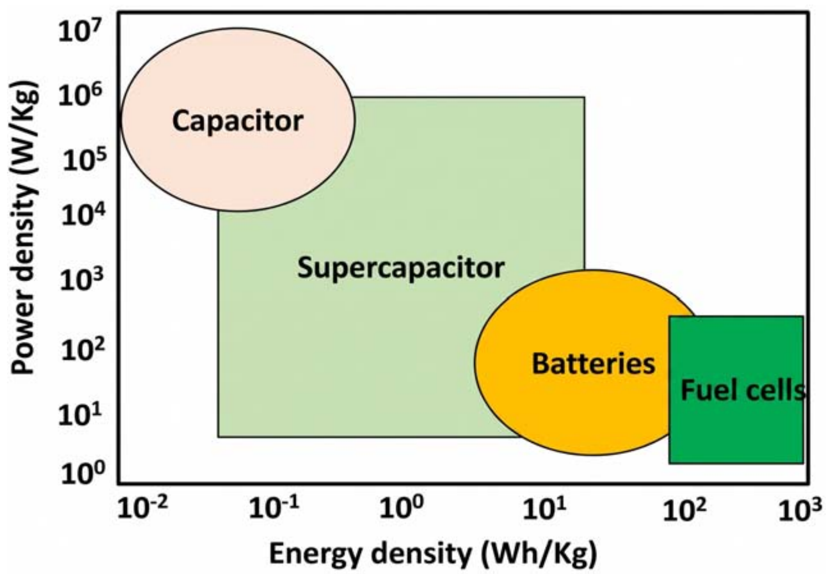

Fig. (1). Ragone plot for different energy systems.

Supercapacitors can be categorized into two primary types based on their mechanisms of charge storage: Electrical Double-layer Capacitors (EDLCs) and pseudocapacitors. In EDLCs, charge storage is achieved through ion electrosorption at the electrode surface, resulting in the formation of an Electrochemical Double Layer (EDL). In contrast, pseudocapacitors store charge *via* faradaic processes, which involve fast and reversible redox reactions [5]. Furthermore, supercapacitors are being combined with intercalation and battery materials in a single electrode configuration to enhance both energy density and power density, as depicted in Fig. (**2a-l**).

The electrode materials used in supercapacitors are typically classified into three main groups: carbon-based materials, transition metal oxides, and conducting polymers. Carbon-based materials, such as Carbon Nanotubes (CNTs), Activated Carbon (AC), and graphene, store charge through the formation of an EDL at the electrode-electrolyte interface, making them suitable for EDLCs [6, 7]. On the other hand, transition metal oxides—such as ruthenium oxide (RuO_2), manganese oxide (MnO_2), and nickel oxide (NiO) and conducting polymers like polyaniline (PANI), polythiophene (PTh), and polypyrrole (PPy) are considered pseudocapacitive materials. These materials exhibit high capacitance due to their ability to undergo rapid redox reactions, contributing to efficient charge storage through faradaic processes [8, 9].

CHAPTER 9

Different Functional 2D Nanocomposites for Charge Storage

Arpita Dutta[1], **Sudip Kumar Saha**[1] and **Abu Jahid Akhtar**[1,*]

[1] *Department of Physics, Diamond Harbour Women's University, West Bengal - 743368, India*

Abstract: The development of effective, affordable, and advanced electrochemical energy storage systems has been a significant challenge for researchers in recent years. The drive to develop improved storage facilities prompted researchers to develop supercapacitors with higher energy density, power density, and cycling life, culminating in the exploration of numerous 2D layered nanomaterials. These materials are widely studied due to their unique physical-chemical properties, enhanced electronic charge transport, high energy storage capability, environmentally friendly, and excellent electrochemical properties, all of which are attributed to their high surface-to-volume relation. Among these materials, graphene, transition metal dichalcogenides (TMDs) like MoS_2, and transition metal carbides, nitrides, and carbonitrides (MXenes) have been extensively researched for their potential applications in supercapacitors. However, the use of these 2D materials in supercapacitors is often limited by the restacking of their layers due to π–π interactions and van der Waals stresses, which reduces the number of active sites. To address this issue, researchers have worked on enhancing the active sites and electrochemical properties of electrode materials by forming nanocomposites with materials that have low resistivity, more active sites, and better thermodynamic stability. In this chapter, the formation of diverse nanocomposites of 2D materials with metal oxides, binary metal oxides, and polymers is discussed, which results in improved electrochemical performance and increased flexibility.

Keywords: Binary metal oxide, Current density, Cyclic stability, Electrochemical performance, Electrode.

INTRODUCTION

The rapid growth of the modern economy, driven by the industrial revolution, population expansion, and rising per capita income, has significantly increased energy demand. The heavy reliance on non-renewable resources like crude oil and coal has led to an energy crisis and intensified the greenhouse effect. The depletion of fossil fuels has motivated scientists to investigate alternative sources

* **Corresponding author Abu Jahid Akhtar:** Department of Physics, Diamond Harbour Women's University, West Bengal - 743368, India; E-mail: abduljahidakhtar@gmail.com

Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma (Eds.)

of energy, such as the sun, wind, and tidewater power, as well as develop efficient energy conversion systems. However, electricity production from renewable sources is often unpredictable, and studies show that inadequate energy storage systems lead to a loss of approximately 30% of generated power [1]. As a result, researchers are focusing on developing sustainable, environmentally friendly, inexpensive, and novel storage systems that have excellent energy and power density [2].

The storage of energy can be accomplished using various methods, including electrochemical, mechanical, potential, and thermal techniques. Of these, electrochemical storage is the most commonly used. Lead-acid batteries, metal-ion batteries (*e.g.*, sodium-ion, lithium-ion) [3], fuel cells [4], and electrochemical capacitors [5]are typical examples of electrochemical storage systems. Among them, batteries have gained widespread industrial use due to their high energy densities, but they face limitations such as low power densities, overheating issues, and shorter cycle life. Conversely, traditional electrolytic capacitors provide high power densities but have limited energy storage capabilities. This difference in performance has motivated substantial research into a new type of energy-storing device named supercapacitors, or electrochemical capacitors [6].

Supercapacitors represent a sustainable and renewable energy storage technology that has attracted significant attention due to their exceptional characteristics, including rapid charging and draining, long cycle life, outstanding power density, and inexpensive, and environmentally friendly nature. These devices operate using electrochemical charging and discharging processes. Supercapacitors are distinguished by their charge-storing mechanisms: EDLCs (Electrical Double-layer Capacitors) and PCs (Pseudocapacitors). EDLCs typically use materials composed of carbon, such as graphene, CNTs (Carbon Nanotubes), and activated carbon, storing energy through ion adsorption and desorption at the interface of the electrode and electrolyte by forming electrochemical double layers. In contrast, PCs rely on materials like conducting polymers, metal oxides, hydroxides, and sulfides, which store energy through fast Faradic electron transfer reactions. Pseudocapacitive materials with multiple oxidation states generally achieve higher energy densities than EDLCs, but their commercial application is limited due to lower electrical conductivity and cyclic instability caused due to poor ionic transfer rates [7, 8].

The diligent choice of the appropriate electrode material is crucial for enhancing the energy density and specific capacitance of supercapacitors. Two-dimensional (2D) layered materials have emerged as promising candidates due to their incomparable electrochemical, optical, and electrical properties. These materials offer significant benefits for subsequent-generation electrochemical devices, including broadened surface area, chemically reactive edge sites, exposed van der Waals gaps for ion intercalation, as well as outstanding mechanical strength and flexibility. Due to its gigantic surface area, robust electrical conductivity, and stable chemical composition, graphene forms the most well-known two-dimensional material [9, 10]. Other 2D materials like TMDs (Transition Metal Dichalcogenides) and MXenes have received large interest for supercapacitor applications. Despite their potential, the gravimetric specific capacitance of 2D materials remains limited due to their low specific surface area and tendency to restack between layers [11, 12].

To overcome these challenges, researchers have been optimizing the surface chemistry and multiscale architecture of 2D nanomaterials to enhance energy storage density and improve electron and ion transport kinetics. One promising approach is the development of composite materials combining metal oxides, hydroxides, and polymers, resulting in hybrid supercapacitors [13, 14]. These hybrid devices combine the benefits of EDLCs and Faradic reactions, offering improved electrical conductivity, multiple oxidation states, larger surface areas, porous structures, and enhanced electrochemical stability, all at a lower cost. In this chapter, we will describe the role of nanocomposite materials in improving supercapacitor performance, making them viable candidates for large-scale applications.

2D NANOMATERIALS FOR SUPERCAPACITORS

Graphene

Since its discovery in 2004, graphene—an allotrope of carbon—has gained significant importance due to its distinct structure and exceptional properties, making it one of the most studied materials today. Graphene is characterized by its two-dimensional honeycomb lattice of sp^2-hybridized carbon atoms, forming a layer just one atom thick, which can be easily derived from graphite.

In the field of electrochemical storage devices, graphene has become prominent thanks to its outstanding attributes: an optimum surface area of 2630 m^2/g, impressive mechanical strength of 1 TPa, rapid intrinsic carrier mobility, excellent electrical conductivity of around 10^6 S/cm, outstanding optical transmittance of 97.7%, and remarkable thermal conductivity of about 5000 W/mK [15]. The exceptional characteristics of graphene are largely influenced by the synthesis methods used, making the selection of an appropriate approach a key challenge in its production. Common techniques for preparing graphene include: chemical vapor deposition, mechanical exfoliation (Scotch Tape Method), chemical decomposition of graphite, solvothermal synthesis, dissolution of carbon nanotubes, epitaxial growth on Si-C surfaces, and liquid phase exfoliation with

CHAPTER 10

PROSpects, Problems, and Future Applications

B. Anil Kumar Naik[1], **Sunil Kumar Singh**[2] and **Awadh Kishor Kumar**[1,*]

[1] *Department of Chemical Engineering and Technology, National Institute of Technology, Patna, Bihar-800005, India*

[2] *Department of Chemical Engineering, BIT Sindri, Dhanbad, Jharkhand, India*

Abstract: The rapid advancement of energy storage technologies has positioned functional 2D nanostructured materials as pivotal in developing next-generation electrochemical devices. This chapter explores the future prospects, challenges, and applications of these materials, emphasizing their role in enhancing supercapacitors, batteries, and fuel cells. The chapter begins by examining the promising prospects of 2D nanomaterials, such as their unique structural properties, high surface area, and exceptional electrochemical performance, which make them ideal candidates for energy storage applications. It explores how these materials can be scaled for commercial use and integrated into flexible and hybrid energy storage systems, paving the way for innovations in portable and wearable electronics. Despite these promising prospects, several challenges hinder the widespread adoption and commercialization of 2D nanomaterials. Environmental and economic implications are also discussed, offering a balanced perspective on the current limitations of these materials. The chapter highlights emerging trends and innovative strategies to overcome these obstacles, including advances in material design, hybrid systems, and large-scale production techniques. The chapter concludes with a discussion on the broader implications of 2D nanomaterials in shaping the future of energy storage, offering insights into their potential impact on the global energy landscape. This chapter serves as a comprehensive guide for researchers, engineers, and industry professionals, providing a clear roadmap for the future development and application of functional 2D nanostructured materials in energy storage technologies.

Keywords: Advanced energy systems, Battery safety, Electric vehicles, Energy storage, Environmental impact, Electrochemical devices, Lithium-ion batteries, Supercapacitors, Scalability, Solid-state batteries, Sustainable technology, 2D nanomaterials.

* **Corresponding author Awadh Kishor Kumar:** Department of Chemical Engineering and Technology, National Institute of Technology, Patna, Bihar-800005, India; E-mail: awadh.ch@nitp.ac.in

Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma (Eds.)

INTRODUCTION

The ongoing energy crisis and the global push for sustainability have fuelled significant advances in energy storage technologies. With renewable energy sources such as solar, wind, and bioenergy becoming more prevalent, the need for efficient, scalable, and reliable energy storage systems is more critical than ever [1]. This necessity arises from the intermittent nature of renewables. Solar power depends on daylight, wind energy varies with weather conditions, and biofuels face challenges in production and consistency [2]. Thus, storing surplus energy during peak production times and releasing it when there is high demand or supply is essential for maintaining a stable and resilient energy grid.

Nanotechnology, particularly nanomaterials, has been at the forefront of the innovation driving advancements in energy storage devices. The unique properties of nanomaterials have allowed researchers to overcome many limitations of traditional materials [3]. From improving the energy density of batteries to enhancing supercapacitors' power output and lifespan, nanomaterials can revolutionize how energy is stored and utilized across industries. The rise of supercapacitors, lithium-ion batteries, and solid-state batteries as efficient energy storage solutions has already demonstrated the critical role of advanced materials [4]. These devices enhance performance metrics such as energy density, power density, and charge-discharge efficiency and pave the way for new applications in areas such as Electric Vehicles (EVs), portable electronics, and large-scale grid storage [5]. For instance, graphene, Carbon Nanotubes (CNTs), and transition metal oxides have emerged as critical materials for improving electrode performance in energy storage systems [6]. Their capacity to store and release energy rapidly, along with their stability under repeated use, makes them ideal for next-generation devices [7].

Despite these exciting advancements, significant challenges remain to the widespread adoption of nanomaterial-based energy storage solutions. To move these technologies from research laboratories into real-world applications, scalability, cost-effectiveness, environmental impact, and long-term stability must be addressed [8]. The economic feasibility of producing nanomaterials at scale and ensuring their life cycle sustainability poses critical questions for researchers and policymakers alike [9]. Furthermore, concerns about the safe handling and disposal of nanomaterials and their potential environmental footprint must be tackled before they can be fully integrated into everyday technologies.

Looking ahead, the future of energy storage will likely be shaped by breakthroughs in multidimensional nanomaterial structures that go beyond the conventional two-dimensional graphene sheets or carbon nanotubes [10]. These materials could unlock unprecedented performance levels through novel fabrication techniques, particularly in energy density and charge rates. At the same time, there is growing interest in combining nanomaterials with other emerging technologies, such as Artificial Intelligence (AI) and machine learning, to optimize energy storage systems and predict performance degradation over time [11].

This chapter explores these issues in detail, focusing on the prospects of nanomaterials for future energy storage solutions, the problems that still hinder their development, and the potential future applications that could change the landscape of global energy infrastructure. We begin by examining the state-of-the-art advancements in nanomaterials for energy storage and discussing how they have pushed the possible boundaries. Following this, the chapter will highlight the primary challenges that need to be addressed for these technologies to realize their full potential. Finally, we will explore emerging applications that could shape the future of energy storage, from smart grids and decentralized power systems to flexible, portable, and even wearable energy storage devices.

Prospects of Nanomaterials in Energy Storage

With the rising demand for more efficient energy storage systems, nanomaterials have garnered attention for their potential to improve device performance significantly. These materials provide unique benefits, including an extensive surface area, excellent electrical conductivity, and adaptable chemical characteristics, which make them highly suited for enhancing energy density, accelerating charge/discharge cycles, and boosting the overall efficiency of batteries, supercapacitors, and other energy storage technologies [12].

Nanomaterials for Enhanced Performance

Nanomaterials possess unique characteristics that allow them to enhance essential performance factors like energy density, power output, and charge cycle durability. Central to these advancements is their high surface area-to-volume ratio, which increases the number of active sites available for electrochemical reactions. This feature facilitates quicker ion movement and enhances charge storage capacity, improving overall performance. Graphene has been one of the most widely researched nanomaterials due to its extraordinary electrical conductivity and mechanical strength. As a two-dimensional material composed of a single layer of carbon atoms, graphene offers a vast surface area that enhances charge storage capacity. Moreover, its flexibility and stability make it suitable for applications in flexible and wearable energy storage devices. For example, graphene-based supercapacitors exhibit high energy and power densities and excellent cyclic stability [13].

SUBJECT INDEX

A

B

C

Sanjeev Verma, Tapas Das, Shivani Verma & Bhawna Verma (Eds.)

D

E

F

G

H

I

L

M

N

O

P

R

S

T

U

V

W

X

Y

Z

Sanjeev Verma

Dr. Sanjeev Verma is an Assistant Professor in the Chemical Science and Technology department at the National Institute of Technology Patna, India. He holds a Ph.D. (IIT BHU), M. Tech. (IIT BHU), and B.Tech. (BTKIT Dwarahat) in Chemical Engineering. Before joining NIT Patna, he worked as a Manager in the Battery Manufacturing Department at Reliance Industries Limited, India. His research interests include: Energy storage materials, Supercapacitors, Batteries, Electric Mobility, Supercapatteries, and Energy storage tech applications.

Tapas Das

Dr. Tapas Das pursued his B.Tech in Chemical Engineering at NIT Rourkela in 2014, followed by M.Tech (2016) and Ph.D.(2022) at IIT (BHU) Varanasi. Then he gained research experience as a post-doctoral scientist at Chonnam National University, South Korea. In 2023, he joined as an Assistant Professor in the Department of Chemical Engineering at NIT Rourkela. He has a keen interest and experience in developing novel composite materials for energy storage devices like supercapacitors, supercapatteries, and batteries. During his post-doctoral research, he developed flexible devices that were useful for smart electronics. He has extended his research to convert biowastes into efficient energy storage materials, generate hydrogen by hydrogen evolution reaction (HER), and develop solar cells. Apart from all these, he is enthusiastic about finding practical solutions to real problems in energy storage and their environmental aspects.

Shivani Verma

Dr. Shivani Verma is an Assistant Professor in the Department of Chemistry at the School of Physical Sciences, Doon University, Dehradun, India. She obtained a Ph.D. degree in chemical sciences division, specialization in organic synthetic chemistry and agricultural chemistry from G. B. Pant University of Agriculture and Technology, Pantnagar, India. Her research interest includes energy storage materials, synthetic chemistry, heterocyclic compounds, heterogeneous catalyst, ionic liquids, green chemistry, agricultural chemistry, and pesticide residue analysis.

Bhawna Verma

Dr. Bhawna Verma is an Associate Professor in the department of Chemical Engineering & Technology at IIT(BHU), Varanasi. She holds a PhD (IIT (BHU), M. Tech. (IT BHU) and B.Tech. (NIT Raipur) in Chemical Engineering. Her research interests include: Advanced Composite/ Nanomaterials for Enhanced Capacitance, Waste Water Treatment, Biodiesel, Catalysis, Heat Transfer in narrow channels. She has authored around 50 research publications, conference papers and book chapters.