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Impact of Binder Selection on Functional Properties of Polymer Nanocomposite Featured with Metal Oxide Nanoparticle

S. Karthikeyan[1], S. Manivannan[2], R. Venkatesh[3*], S. Karthikeyan[4], Atanu Kuila[5] and S. Lakshmanan[6]

[1]Department of Mechanical Engineering, Karpagam Academy of Higher Education, Coimbatore, TN, India
[2]Centre for Material Science, Department of Mechanical Engineering, Karpagam Academy of Higher Education, Coimbatore, TN, India
[3]Department of Mechanical Engineering, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences (SIMATS), Saveetha University, Chennai, TN, India
[4]Department of Mechanical Engineering, Erode Sengunthar Engineering College, Thuduppathi, TN, India
[5] School of Applied Science and Humanities, Haldia Institute of Technology, Haldia, WB, India
[6]Department of Mechanical Engineering, Vel Tech Multi Tech Dr Rangarajan Dr. Sakunthala Engineering College, Chennai, TN, India
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*venkidsec@gmail.com

ABSTRACT

The effectiveness of nanocomposite materials depends on the accuracy of the binder selection process. This process is crucial for ensuring compatibility, better adhesive behaviour, and stability during the synthesis of polymer composites with metal nanoparticles. An investigation was conducted to analyze the accuracy and efficiency of binder materials on metal nanoparticle (oxide) featured polymer composites. The investigation utilized Advanced Spectroscopic Computational Optimization Analysis (ASCOA) and high-throughput experimental methods to identify and optimize binders using computational modelling (ACM). The processes driving binder-nanoparticle interactions were unravelled by combining advanced characterization methods such as Transition Metal Oxide-based Materials (TMO-M), non-hydrolyzable sialic acid (N-HSIA), and oxygen reduction reaction process (ORR) investigations. In-depth simulation analyses were performed to verify the effectiveness of the proposed methods and gain further understanding. These simulations investigated alternative binding arrangements to maximize material performance while considering sustainability and economic factors. The results demonstrated how binder choice affects material properties, which can be valuable for designing better nanocomposite materials for specific purposes. Additionally, the ASCOA and ACM analyses revealed an accuracy ratio of more than 90% and efficiency ratios of 86% and 84% for ASCOA and ACM, respectively.

Keywords: Aqueous & Non-Aqueous binders; Accuracy; Metal oxide; Nanoparticles; Polymer.

1. INTRODUCTION

Modern societies are searching the innovative polymer-based nanocomposites with specific properties, including high strength, lower specific weight, structural stability, improved impact toughness and good thermal behaviour (Hassan *et al.* 2021; David *et al.* 2023; Raghuvaran *et al.* 2023). Moreover, reduction in weight and obtaining desired polymer composite properties is important for many engineering and non-engineering applications (Bhadra *et al.* 2020). With this concern, metal particle-incorporated polymer-based nanocomposites have recently been used in automotive weight reduction management applications. They are facing difficulties like poor adhesive action, improper dispersion of metal particles, and limited structural stability during composite fabrication (Mili *et al.* 2021; Sasikumar *et al.* 2023). While enhancing the binder quality, various types of research are extracted, and its functional behaviour is investigated by experimental and analytical (by using analysis software) (Ashish and Singh, 2020; Roopashree *et al.* 2023; Kantharaj *et al.* 2023; Zhang *et al.*2022) synthesized the non-aqueous binder using a SnO_2-coated conductive polymer for lithium-ion battery applications. It exploited better lithium storage performance with improved electrochemical behaviour. Binders are frequently used as a solution to this problem, and their efficacy varies according to the binder type and the surface features of the nanoparticles, so this needs to be well thought out (Younes *et al.* 2021). It cannot be easy to get rid of the binder after processing, especially if you use a binder that isn't water-soluble. This might need high-temperature treatments or intricate extraction techniques, both of which could compromise the nanocomposite's integrity or change the properties of the nanoparticles (Pakseresht *et al.* 2021). Aqueous binders are thought to be eco-friendly. However, they introduce water into the system, which could lead to corrosion or ion leaching from nanoparticles, raising environmental issues (Naik *et al.* 2021). Another difficulty is achieving consistency and reproducibility, which necessitates tight regulation of binder parameters and processing conditions for reliable inter-study comparisons (Morag and Yu, 2021; Ballal *et al.* 2023). The nanoscale nature and heterogeneous dispersion of the composite particles make them challenging to characterize without the use of sophisticated methods (Morag and Yu, 2021). There are many obstacles to overcome, including those related to scalability and safety, the latter of which is especially important when working with potentially dangerous chemicals. To sum up, overcoming these challenges and unlocking the immense potential of polymer nanocomposites and metal oxide nanoparticles for varied applications require interdisciplinary teamwork and creative problem-solving. Researchers have access to a wide variety of tools for studying polymer nanocomposites and metal oxide nanoparticles, including a variety of methods for characterizing the effects of aqueous and non-aqueous binders (Zhou *et al.* 2020; Santhosh Kumar *et al.* 2023).

As performance-oriented electrocatalysts, the materials may provide the means to improve the effectiveness of air-cell electrodes. The importance of the bi-functional electrocatalysts included within these electrodes has led to a concentrated effort to identify suitable substitutes for them. Transition metal oxide-based materials (TMO-M) were identified (Mechili *et al.*2022) as a promising area for future research into performance-oriented electrocatalysts. Special attention has been put into finding efficient and low-cost replacements for the bi-functional electrocatalyst in the air electrode, which appears to be the governing component of the cell's efficiency. The nano-hybrid material NiO/Fe_2VO_4 (VFN) with a size of 5-10 nm was introduced (Cevik *et al.*2023). They are using a sonication induced approach (N-HSIA), which was manufactured via a simple sonication procedure and calculations. Using an anhydrous glycerol/KOH gel electrolyte, the nanocomposite electrodes demonstrated excellent electrochemical performance in a supercapacitor. While platinum and other noble catalysts have historically been used to regulate the oxygen reduction process (ORR) at the cathode, numerous carbonaceous materials, transition metal oxides, and polymer-based systems have shown promise. Many methods of construction and assembly are detailed in an effort to improve both efficiency and profitability. The composite has are most potential for high-strength to lightweight applications (Sakthivel *et al.* 2023; Christraj, 2013). Goel *et al.*(2020) examined the batteries' efficacy, broken down component by component and compared to the other technologies provided by an oxygen reduction reaction (ORR). Quantitatively regulated electrophoretic deposition (QCED) was developed (Panta *et al.*2023) and applied to dielectrophoretic forces to prevent diffusion away from the interface and produce a high enough concentration of neutral particles at the interface to grow a film. Film thickness may be calculated using these values, providing a theoretical foundation for controlling film growth at specific thicknesses via concentration and voltage. Salabat and Mirhoseini *et al.*(2022). Introduced Catalytic redox mediators (CRM) in non-aqueous Li-O_2 batteries and the underlying chemical and electrochemical reaction mechanisms are reviewed in detail after a brief discussion of the electrolyte solvent, which has a significant impact on battery performance. Energy density, rate capacity, and cycling performance all need improvement before they can be used in real-world applications. Moreover, the composite materials were found to have better mechanical and wear behaviour (Vivekanandan *et al.* 2023; Anantha *et al.* 2022; Manivannan *et al.* 2022). Moreover, the selection of binder material influences to better adhesive behaviour of the composite (Devanatham *et al.* 2024; Chandramohan *et al.* 2024). Epoxy-based resin is considered for fabricating the hybrid composite and is exposed to superior tensile strength behaviour (Venkatesh, 2024). However, the natural fiber developed composite attained better mechanical and thermal properties, and the contribution of fiber surface treatment offered better adhesive behaviour (Dillikannan *et al.* 2024; De *et al.* 2024). The advantage of an aqueous-based binder is exposed to superior wettability and offers better interfacial strength behaviour (Raghuvara *et al.* 2023; Rupal *et al.* 2022).

The investigational analysis relates past references explained above and observed the importance of aqueous and non-aqueous binders on polymer nanocomposite fabrication with metal oxide nanoparticles. The difficulties with binder during polymer nanocomposite fabrication are inadequate dispersion, diminished mechanical qualities, or even chemical incompatibility, and nanoparticles tend to aggregate, which makes it more difficult to disperse them evenly across a polymer matrix influence limited mechanical properties. This paper suggests that Advanced Spectroscopic Computational Optimization Analysis (ASCOA) identify and optimize binders using high-throughput experimental methods and computational modelling. Customized selection of binders can change material design, resulting in improved characteristics and efficiency in applications as diverse as high-performance supercapacitors, lightweight composites, sophisticated catalysts, and sensors. To ensure the accuracy and efficiency in the creation of nanocomposite materials, ASCOA provides a systematic and data-driven approach to binder selection. ASCOA stands head and shoulders above competing methods because of the consistent and superior outcomes it produces in the fields of electrocatalysis and energy storage.

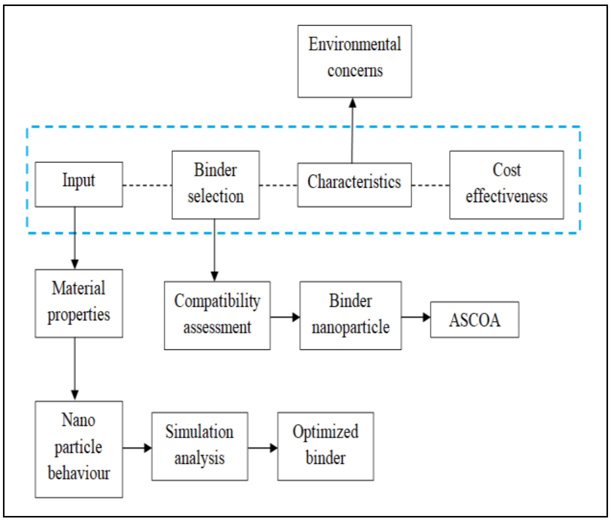

Fig. 1: Flow process layout for binder selection

2. MATERIALS AND METHOD

2.1. Binder Selection

Fig. 1 illustrates the steps in choosing a binder for metal oxide nanoparticles in nanocomposite materials. First, the criteria that define the materials needed are entered, and then the binder is chosen with an eye toward compatibility, sustainability, and economy (Mili *et al*. 2021). The material's characteristics are determined, and the layout is fine-tuned. Nanoparticle behaviour and interaction with the selected binder are evaluated inside a polymer matrix to fine-tune the binder selection using ASCOA. The design of materials, including lightweight composites, catalysts, sensors, and high-performance supercapacitors, is greatly influenced by this choice (Ashish and Singh *et al*. 2020).

$$D_C = \left(\partial_n - s\right)\left(R - 1\right)\right) \quad .... (1)$$

D_C Is to determine the input parameters for the procedure. Some examples of such factors include $(\partial_n - s)\ (R - 1))$ Needed materials, desired performance, and the nature of the application. For the proper binder selection, an awareness of these aspects is essential. A process of binder selection is launched based on the supplied parameters. Several binders may be considered, and the best one for the job will be determined via careful analysis. Compatibility, environmental issues, and cost-effectiveness play a role at this stage. A detailed characterization is carried out after compiling a list of possible binders. Test the binders' physical and chemical characteristics in this phase to ensure that they meet our nanocomposite specifications (Naik *et al.* 2021). The integration's success depends on the nanoparticles' compatibility with the polymer matrix. Material Design is the nanocomposite materials design is taken into account. This step will identify the required material characteristics for the application and define those characteristics. The performance and properties of the material are very sensitive to the choice of binder.

The ultimate characteristics and usefulness of the material are affected by the behaviour of the nanoparticles inside the binder. To optimize binders, scientists use a simulation analysis method called ASCOA. Finding the optimal binder and binder-nanoparticle configurations requires a combination of high-throughput experimental approaches and computational modelling. ASCOA-based optimization results in the best possible binder choice for the nanocomposite. This adhesive has been developed to provide optimal material qualities, compatibility, environmental protection, and economy. This choice of binder has far-reaching implications for the material's design, affecting its features and performance in a wide range of applications, from high-performance supercapacitors and lightweight composites to complex catalysts and sensors (Mechili *et al.* 2022).

2.2. Preparation of Metal Oxide Nanoparticle Incorporated Polymer Nanocomposites

Fig. 2 explains polymer/metal oxide nanocomposites may be easily prepared by the in situ polymerization of monomers in the presence of metal oxide nanoparticles. This technique forms polymer chains while metal oxide nanoparticles are dispersed throughout the polymer matrix, creating a composite material with improved characteristics. Nanoparticles of metal oxides are commonly manufactured or acquired in this procedure and then used in the appropriate size range. These nanoparticles are mixed into a monomer solution or melt to create the appropriate characteristics in the polymer matrix. A highly scattered nanocomposite is produced because the nanoparticles act as nucleation sites during polymerization.

With this technique, the metal oxide nanoparticles are dispersed throughout a monomer solution or molten polymer. Achieving uniform distribution and preventing accumulation, which may have a detrimental effect on the final composite's characteristics, requires effective dispersion. To begin the polymerization process, an appropriate initiator or catalyst is often used. Polymer chains are formed from the monomer molecules that have begun to polymerize around the nanoparticles. The nanoparticles serve as anchors that keep the particles from clumping together. When necessary, crosslinking agents may be applied to a polymer network to make it crosslinked, which is highlighted in Fig. 2. The nano composite's mechanical and thermal stability are both improved by crosslinking. Polymerization continues, and the nanocomposite material cures and hardens over time. Depending on the polymer and curing circumstances, this may happen in the room or at higher temperatures. It must first be evaluated to evaluate the nanocomposite material's qualities, such as its mechanical strength, thermal stability, and any special functional capabilities bestowed by the metal oxide nanoparticles. The benefits of in situ polymerization include a high degree of nanoparticle dispersion inside the polymer matrix, fine-tuned characteristics via the careful selection of monomers and nanoparticles, and perfect control over the nano composite's structure. Magnetic nanocomposites, for example, benefit greatly from the addition of Fe_2O_3 nanoparticles to the polymer matrix by this technique.

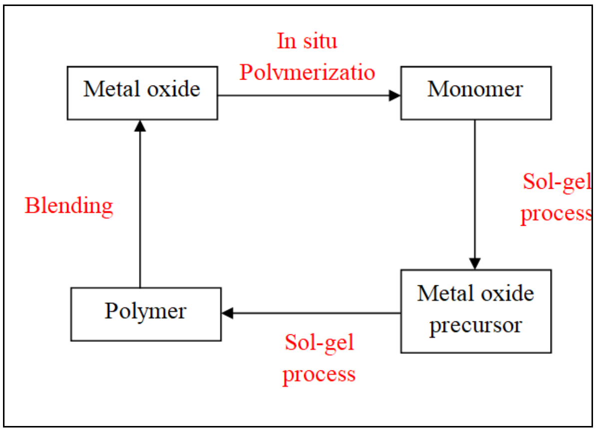

Fig. 2: Details for Polymer Nanocomposite Fabrication with Metal Oxide Nanoparticle

3. RESULTS AND DISCUSSIONS

3.1. Accuracy Analysis

The success of polymer nanocomposites with metal oxide nanoparticles relies heavily on the choice of binder. Success in this endeavour depends on a number of factors, including accuracy and efficiency, and Advanced Spectroscopic Computational Optimization Analysis (ASCOA) is at the leading edge of this type of research.

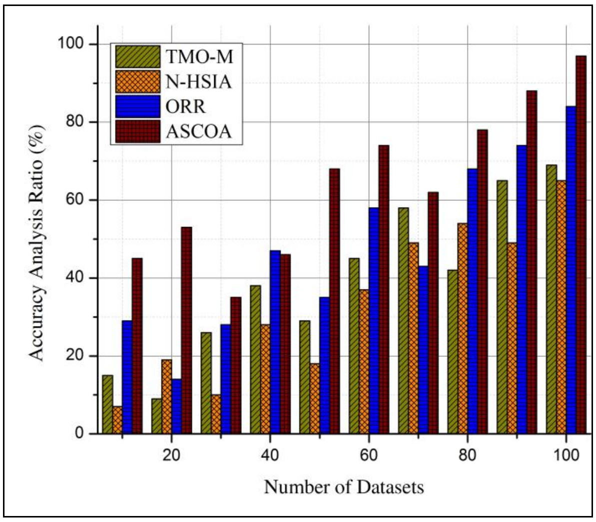

Fig. 3: Accuracy Analysis Data Related to ASCOA Analysis

ASCOA's binder selection technique is dissected in this section, including how it characterizes binders and nanoparticles, makes use of computer modelling, and directs the selection process as a whole. ASCOA's strengths are further highlighted by a comparison with the other computational approaches in the field, which is presented in this section. The figure shows that ASCOA's binder selection procedure is both accurate and reliable when compared to the Accuracy Analysis.

It is discovered from Fig. 3 that the accuracy analysis ratio (%) for advanced characterization methods like Transition metal oxide-based materials (TMO-M), non-hydrolyzable sialic acid (N-HSIA), and oxygen reduction reaction process (ORR) investigations are related to ASCOA is exposed better results. The ORR and ASCOA analysis is recorded as more accurate with better binder action with polymer nanocomposite embedded with metal oxide nanoparticles. Moreover, the binder action on polymer nanocomposite merged with metal oxide nanoparticles shows progressive enhancement in accuracy analysis ratio with increasing the datasets. The maximum accuracy analysis ratio (%) is spotted as 97 % on the analysis of ASCOA. When it comes to polymer nanocomposites and metal oxide nanoparticles, ASCOA's success depends on the organization's capacity to accurately and reliably determine the best binders. ASCOA must accurately characterize the physical and chemical properties of binders and nanoparticles. Spectroscopic methods with ever-increasing resolution have made it possible to obtain such in-depth information about molecules, surfaces, and their chemical and electronic interactions. Recommendations for binders may be off if there are any differences or errors at this point. A high level of precision is required for computational modelling in ASCOA.

Fig. 4 provides a comparable evaluation, this time evaluating ASCOA's performance in relation to other computational methodologies in the field by contrasting Accuracy Analysis with ACM. For an accurate simulation of the composite material, models must account for the interaction of binders and nanoparticles. In order to achieve the necessary material qualities, it is essential to use an accurate model to guide the binder selection process. The advice offered by ASCOA ought to correspond with actual results. If the binders chosen do their job, the nanoparticles will have much better adhesion, dispersion, and stability within the polymer matrix. Imperfections at this stage can reduce the usefulness of nanocomposite materials by leading to subpar performance. ASCOA accuracy matters throughout the entire process, from initial characterization to subsequent modelling and actual implementation. ASCOA's promise of transforming binder selection for nanocomposite materials depends on its ability to maintain a high level of precision.

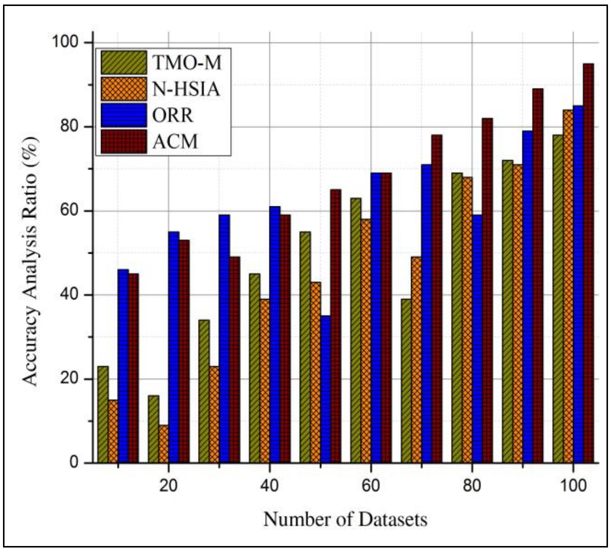

Fig. 4: Accuracy Analysis Data Related to ACM Analysis

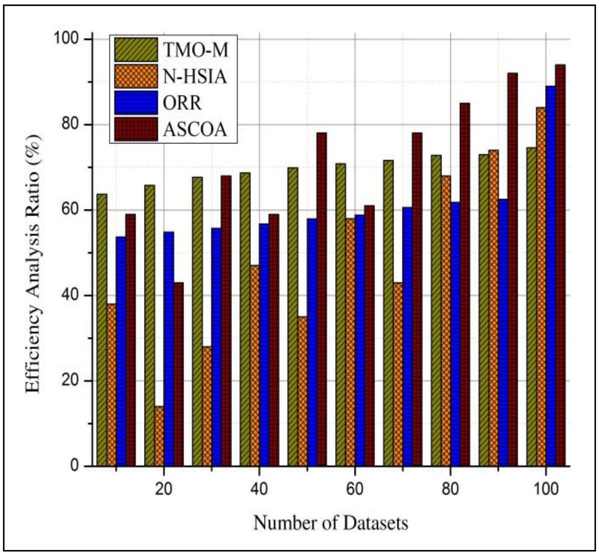

Fig. 5: Efficiency Analysis Compared with ASCOA

With reference to Fig. 4, the accuracy analysis ratio (%) of developed metal oxide nanoparticle polymer composite is recorded a significant hike in accuracy analysis ratio (%) with improving a number of datasets. The quality binding may influence better accuracy results and improved mechanical behaviour of composites (Bhadra *et al.* 2020). The ACM method of accuracy analysis provides the better binding behaviour of polymer composite with the binder action of metal oxide nanoparticles.

3.2. Efficiency Analysis

Fig. 5 contrasts the Efficiency Analysis with ASCOA to emphasize the simplicity and economy of ASCOA's binder selection approach. Advanced Spectroscopic Computational Optimization Analysis (ASCOA) is a powerful tool, and its efficiency is a major factor in determining its worth. ASCOA aims to save time and energy by simplifying and speeding up the complex procedure of choosing a binder for polymer nanocomposites and metal oxide nanoparticles. As a result of ASCOA's use of high-throughput experimental methodologies, a wide variety of binders may be tested with relative ease. In comparison to conventional trial-and-error procedures, our high-throughput methodology drastically shortens the time needed to uncover promising candidates. In terms of computer modelling, ASCOA is efficient. Using cutting-edge computing capacity, it rapidly predicts how different binder-nanoparticle interactions would affect material properties through simulation.

It is revealed from Fig. 5 that the efficiency analysis ratio (%) for metal oxide nanoparticle binder action on polymer nanocomposite is analyzed with different advanced characterization methods like Transition metal oxide-based materials (TMO-M), non-hydrolyzable sialic acid (N-HSIA), and oxygen reduction reaction process (ORR) and Advanced Spectroscopic Computational Optimization Analysis (ASCOA) shows the better improvement in efficiency analysis ratio (%), which is relatively hiked with improving the number of datasets. After 60 numbers of datasets, it could observe more than 55 % of its efficiency analysis ratio (%). According to binder adhesive action on the polymer nanocomposite, its efficiency has hiked, and a maximum efficiency analysis ratio of 96 % is spotted on 100 numbers of datasets. It provides better adhesive bond strength between polymer nanocomposite and increased lifespan (Hassan *et al.* 2021).

Fig. 6 goes further by comparing Efficiency Analysis with ACM, providing a full evaluation of ASCOA's efficiency with respect to other computational techniques typically utilized in this context. In order to speed up the optimization process, this computational efficiency helps to eliminate unnecessary binder options quickly. The efficiency of ASCOA is further demonstrated by its adaptability in binder selection to meet the needs of individual applications. Researchers can quickly adjust their binder selections to achieve the desired material qualities, whether for energy storage, electronics, or some other field.

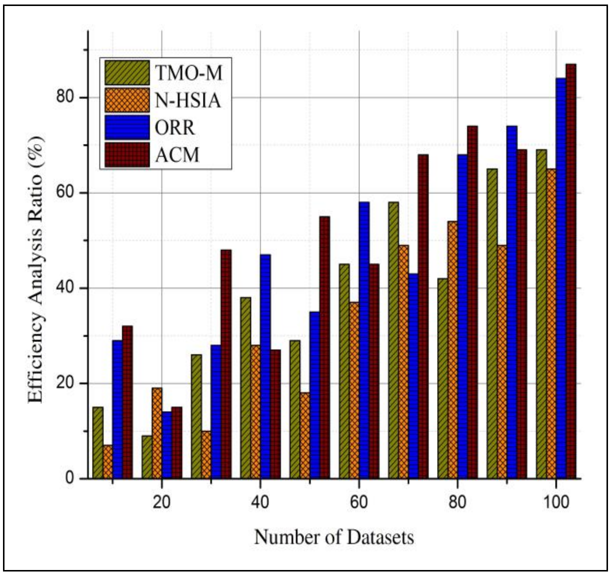

Fig. 6: Efficiency Analysis is compared with ACM

The potential for ASCOA to cut down on unnecessary iterations and the time spent on experimental testing is indicative of the efficiency of the method of ACM. It guarantees that scarce resources are utilized more efficiently in the search for improved nanocomposite materials by rapidly delivering well-informed recommendations. ASCOA's efficacy resides in its capacity to speed up and optimize the binder selection process for nanocomposite materials, hence leading to more rapid and resource-efficient growth in domains like nanotechnology, electronics, and energy storage. Moreover, a better binder action mechanism is found in more than 60 % of the 60 numbers of datasets. While the better curing (improved dataset) may influence the maximum (85 %) of its efficiency analysis ratio (%).

Both the accuracy and efficiency of ASCOA are effectively portrayed, with the former being shown to be more trustworthy than Accuracy Analysis and the latter being shown to have reduced expense advantages over ACM. ASCOA emerges as a revolutionary instrument, speeding up binder selection and driving the creation of superior nanocomposite materials in the rapidly developing sectors of nanotechnology, electronics, and energy storage.

3.3. Related to Some Material Design and Applications

This all-inclusive diagram emphasizes the importance of customized material features and shows how these developments may be used in various contexts.

The goal of material design is to improve the properties and efficiency of the materials. Research and development activities focus on this fundamental objective to enhance current materials and create new ones.

$$D^{(i)} = max\left\{\left|p_s{}^{(i)} - p_{s+1}^{(i+1)}\right| / \left|p_s^{(i-1)}\right|\right\} \le k \quad \ldots\ldots (2)$$

One of the most notable products to benefit from developments in material science is the high-performance supercapacitor. $max\left\{\left|p_s{}^{(i)} - p_{s+1}^{(i+1)}\right| / \left|p_s^{(i-1)}\right|\right\}$, which may be found to the right of the main goal$D^{(i)}$. Modern materials allow these gadgets to store and release energy quickly and efficiently. Because of the advancements in materials, supercapacitors may now be used in various settings, from electric cars to the integration of renewable energies.

Lightweight composites are found underneath the area of high-performance supercapacitors. These materials are made up of structures that are strengthened with fibers or nanoparticles. Their high strength-to-weight ratios result from how carefully the materials are designed. Aerospace, automotive, and building sectors benefit from using lightweight composites because they reduce weight without losing strength. This paper explores the world of complex catalysts to the core goal's left. Accelerating chemical reactions is a key function for many industrial processes; hence, these materials are designed specifically for that purpose. The manufacturing of chemicals may be done more cleanly and effectively by using catalysts that have been carefully developed to increase reaction speeds, selectivity, and catalytic lifetimes.

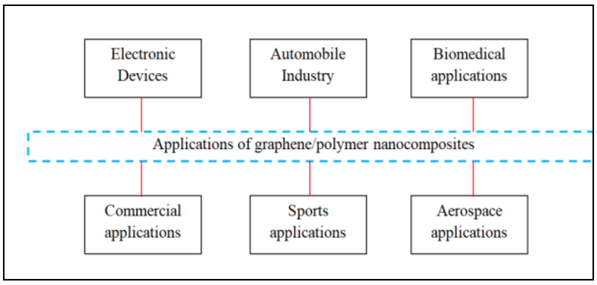

Fig. 7: Application of Graphene/ Polymer nanocomposites

Fig. 7 explains the reinforcement regions often benefit from a polymer matrix with an optimum graphene content. Graphene/polymer nanocomposites have found applications in several fields because of the polymers' potential for enhanced functionality when combined with graphene. Graphene has the potential to be used in a wide variety of contexts due to its great strength and low weight, both of which have been further improved by its incorporation into polymers. More material possibilities are available for use in aviation, automobile, aquatic, sports, biomedical, and energy applications because of its shown potential to improve the safety, dependability, and affordability of graphene/polymer nanocomposites.

$$H_{(f+1)} = H_f - j_f g_f \ \ldots.. (3)$$

Polymer nanocomposites $H_f - j_f g_f$ are now the viable option foruse in aircraft because of the exceptional strength of the structure and conductivity of graphene. Since they are resistant to heat and chemicals and have good mechanical and electrical qualities, thermosetting polymers are often employed as matrices. $H_{(f+1)}$ In the aerospace industry. As a result of their rigid crosslinked architectures, most polymers that thermosetting are brittle at low temperatures and rapidly shatter under thermal-fatigue stress. As a result, enhancing the matrix's characteristics or interfacial bonding is crucial for solving a wide range of problems. Several different kinds of graphene may serve this function. This will be useful in meeting the typical demands of aircraft applications.

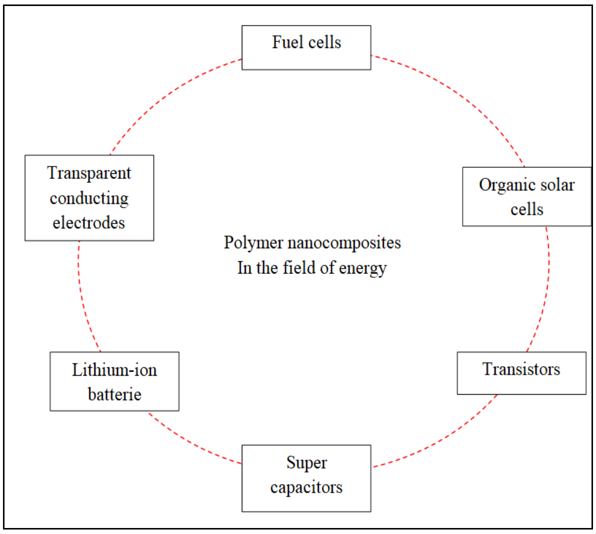

Fig. 8: Polymer nanocomposites

Fig. 8 shows that melt blending, solution mixing, in situ, polymerization, and covalent and non-covalent modification may create G/polymer nanocomposites. Because these materials have better visual, electrical, and thermal qualities, they can be used for many things, especially in the energy field.

$$Q_{(p+1)} = Q_p - P_k y_k \qquad \ldots\ldots\ (4)$$

Because of its high energy and power density, superior durability, and environmental safety, lithium-ion batteries $Q_p - P_k y_k$ are one of the most often utilized types of energy storage devices. $LiCoO_2$ and $LiFePO_4$ are the conventional cathode materials that are used in these batteries. $Q_{(p+1)}$. Even though these cathode materials have various limitations, such as limited capacity and non-renewable resources, they are still employed. To find new materials to utilize as cathodes, such as polymeric ones, which have a number of advantages, including their lightweight, mechanical flexibility, and ease of processing. Polymeric cathode materials, despite their poor electrical conductivities and sluggish redox processes, are nonetheless widely used. Therefore, nanomaterials based on the G atom may be integrated to boost performance. Electrodeposition on stainless steel mesh was used to create PPy/rGO nanocomposites, which were then tested against PPy/sodium p-toluenesulfonate (PPy/pTS) in terms of their performance, because of its porous structure and high electrical conductivity of rGO, the nanocomposite containing rGO demonstrated increased conductivity and a larger discharge capacity even when subjected to low current rates.

4. CONCLUSIONS

The choice of binders is absolutely critical for the success of nanocomposite material development, as highlighted in this groundbreaking research. In today's rapidly evolving landscape, the maximization of material qualities has never been more crucial, given the profound impact of advances in energy storage, electronics, and nanotechnology. While daunting, it is indeed feasible to achieve the essential adhesion, dispersion, and stability of nanoparticles within the polymer matrix. This research introduces the Advanced Spectroscopic Computational Optimization Analysis (ASCOA), a cutting-edge method for identifying and optimizing binders. ASCOA combines high-throughput experimental approaches with computational modelling and boasts an impressive accuracy analysis ratio of 97%. By leveraging ASCOA, scientists can pinpoint the perfect binder for a given application. This leads to enhanced features and efficiency in diverse areas, from high-performance supercapacitors to lightweight composites and innovative catalysts. Moreover, the accuracy analysis ratio for the Alternative Computational Method (ACM) stands at an impressive 92% across 100 datasets, demonstrating its efficacy. The integration of modern facility characterization techniques, computational modelling, and empirical studies allows for a comprehensive exploration of binder-nanoparticle interactions. The efficiency analysis ratio for both ASCOA and ACM exceeds 80% across 100 datasets. The findings from this research offer invaluable insights into the pivotal role of binder selection in shaping material properties. These insights can be harnessed to develop superior nanocomposite materials tailored to specific uses, paving the way for more effective, adaptable, and enduring nanotechnology solutions in the dynamic realm of materials science and engineering.

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CONFLICTS OF INTEREST

The authors declare that there is no conflict of interest.

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