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Optimization and Characteristics of Multimodal Binder on Polymer Nanocomposite for Lightweight Applications

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ABSTRACT

The process of selecting binders is complex because it requires finding a balance between improving material performance and reducing environmental impact. This involves challenges such as achieving nanoparticle dispersion, optimizing binder compatibility, and addressing environmental concerns. The main objective of this research on use the multimodal binder optimization characterization model (M-MBOCM) analysis to understand the intricate relationship between metal oxide nanoparticles, polymer matrices, and binders. These specialized nanocomposites have a wide range of potential applications. By intelligently selecting Scanning Characterization binders (SCB), industries can enhance material properties to meet specific requirements. This applies across various fields, from high-capacity energy storage devices to lightweight structural materials and smart sensors. This research involves analyzing metal oxide nanoparticle mage polymer nanocomposites with aqueous and nonaqueous binders in manganese dioxide-based cathodes (M-BC), hybrid supercapacitors (HS), and non-enzymatic glucose sensors (NEGS). The significance of M-BC in the present investigation results is based on advanced M-MBOCM and SCB techniques. The performance analysis ratio exceeds 95%, which is higher than the reported results for M-BC, HS, and NEGS. The scalability analysis ratio for M-MBOCM and SCM is observed to be higher than others, recorded at 93% and 88% respectively. These findings demonstrate the potential for enhanced nanocomposite materials in practical applications (lightweight) and drive their development.

Keywords: Aqueous/Nonaqueous binder; Nanocomposite; Performance; Polymer; Scalability.

1. INTRODUCTION

Hybrid composites are specialized in engineering applications and expose superb mechanical, thermal, and wear behaviour (David et al.2023; Manivannan *et al.* 2022). The polymer-based nanocomposites are advantageous over the monolithic polymer and own specific strength, better stability, improved toughness, high corrosion resistance, and economic regard. It is widespread in various engineering and non-engineering applications (Hassan et al.2021). The metal oxide nanoparticle incorporated polymerbased nanocomposite materials are attracted in lightweight automotive components, thermal management electronic components, packing, battery and supercapacitor applications (Zadehnazari, 2023; Hussain et al. 2020). Specifically, the metal oxide nanoparticle incorporated polymer nanocomposite composite materials are the best choice for energy sector applications and to enrich the performance of batteries and supercapacitors (Patil et al. 2022). Metal oxide nanoparticles in polymer nanocomposites with aqueous and nonaqueous binders present a number of significant issues and complications that need to be addressed in this developing area of materials research (Balasubramaniam et al. 2020). One of the most important challenges is keeping the metal oxide nanoparticles dispersed and stable within the polymer matrix (Leong et al. 2022; Christraj, 2013). Hybrid reinforcement influences better functional behaviour of composite (Roopashree et al. 2023).

Nanoparticle agglomeration can reduce the benefits of using them in composite materials by preventing them from being fully distributed throughout the material (Xie et al. 2020; Kantharaj et al. 2023). It's not easy to find a binder that works for this agglomeration issue. Additionally, it's a conundrum whether to use aqueous or nonaqueous binders. Although aqueous binders are eco-friendly, they still introduce water into the system, which might increase the risk of corrosion and reduce the stability of the nanoparticles (Wang et al. 2021). On the other side, nonaqueous binders might have

environmental effects and complicated extraction methods.

Furthermore, there are problems with compatibility when picking binders (Zou et al. 2020). The binder has to be suitable for both the polymer matrix and the metal oxide nanoparticles. Chemical reactions caused by incompatibility can change the nanoparticle characteristics or jeopardize the composite (Liang et al. 2022). Binder removal post-processing is a significant hurdle that can't be ignored. In the case of nonaqueous binders, in particular, damaging or otherwise altering the material may be necessary due to the need for hightemperature treatments or complex extraction operations (Zhang et al. 2021). The issues of standardization and reproducibility are quite important (Ballal et al. 2023; Vivekanandan et al. 2023).

Consequently, results from multiple studies may be compared, and researchers need to create standard protocols for binder selection, concentration, and processing conditions (Javed et al. 2023). Several obstacles need to be overcome, as shown by the examination of metal oxide nanoparticles in polymer nanocomposites with aqueous and nonaqueous binders. Maintaining repeatability in the face of the challenges of spreading, stabilizing, and being environmentally compatible is typical in this area of study (Otgonbayar et al. 2023). Solving these problems is essential for realizing the full promise of these materials in fields as diverse as electronics and advanced materials. The production and characterization of materials containing metal oxide nanoparticles have been approached using a number of established methods and tools. The use of such methods is not without its difficulties, though. The size and composition of nanoparticles can be precisely controlled by using techniques such as sol-gel and hydrothermal production (Chakrabarti et al. 2022; Anantha et al. 2022).

In an effort to design a cathode material that is suited for Zn2+ intercalation, (Yadav et al. 2023) came up with the idea of manganese dioxide-based cathodes (M-BC). This review provides an overview of all the mechanisms that are associated with the various polymorphs of MnO₂ cathode. This overview additionally includes an examination of the challenges that are faced by cathodes, anodes, and electrolytes, as described above. The energy storage process in the hybrid supercapacitors (HS) developed (Chatterjee and Nandi, 2021) and discussed in detail, including the contributions of non-faradic electrical double-layer capacitance and faradaic pseudo-capacitance to the total capacitance. Challenges in real-world applications and the potential for future work are discussed, along with the state-of-the-art future applications of supercapacitors in robotics, renewable and sustainable energy devices, wearable and self-healing supercapacitors, and biotechnology. The unprecedented need for highly efficient, stable, selective, and sensitive detection of glucose in the blood and fluids led to the development of non-enzymatic glucose sensors (NEGS) (Naikoo et al.2021). Nanomaterials' aspect ratio, surface shape, active sites, architectures, and catalytic activity have been investigated. All these factors play a crucial part in the development of effective NEGS. For 2D materials to advance in the fields of energy storage and conversion, Xu et al.(2019) designed covalent organic frameworks (COFs). Achieving peak performance from such gadgets depends heavily on the electrode materials used. This has inspired us to contribute to a road map on twodimensional materials for energy storage and conversion. Aqueous zinc-ion batteries (AZIBs) have been studied by layer-structured hydrated vanadium oxides (L-SHVO), where one of the challenging issues is the relatively narrow interlayer spacing (4.4 for (0 0 1) plane) and the poor electronic conductivity that typically leads to the sluggish Zn2+ ions/electrons transport kinetic and the instability of structure, resulting by incorporating polyaniline macromolecules to control the interlayer spacing and structure stability, have discovered a powerful "one for two" technique or the creation of highperformance cathodes for AZIBs and perhaps other multivalent ion storages. The ultimate goal of all of these studies is to improve upon current methods and equipment. A focus on better efficiency, steadier operation, and more varied uses motivates the development of Multimodal Binder Optimization Characterization Modelling (M-MBOCM). The goal of these efforts is to not only address pressing issues of the present but also pave the way for groundbreaking innovations in fields such as robots, renewable energy, wearable technologies, and biotechnology (Liu et al. 2020).

Incorporating metal oxide nanoparticles into polymer nanocomposites presents numerous challenges, including the need for meticulous control of reaction conditions, potential contaminants, and achieving uniform dispersion of nanoparticles in the polymer matrix. The selection of the appropriate binder is paramount to ensure the even distribution of nanoparticles across the matrix. Previous research has highlighted the widespread use of aqueous and nonaqueous binders, each posing distinct challenges related to compatibility, environmental impact, and postprocessing removal. The main objective of the research is to gain a comprehensive understanding of the critical role binders play in nanoparticle incorporation, including their impact on dispersion, compatibility, and ecological considerations and contribution as the major material for the best interaction between the matrix and fiber/filler material. This study aims to unravel the intricate interplay between binder types, polymer matrices, and nanoparticles, all of which significantly impact material performance. Our research recommends the utilization of Multimodal Binder Optimization Characterization Modeling (M-MBOCM) and Scanning Characterization

binders (SCB), supported by compelling evidence that underscores their effectiveness. Through in-depth analysis of performance and scalability ratios across diverse datasets, we aim to offer flexible solutions applicable across various sectors while ensuring exceptional material performance.

2. MATERIALS AND METHOD

In this study, Metal Oxide Nanoparticles (MONPs) are extensively studied as fillers in polymer nanocomposites using either aqueous or nonaqueous binders. Moreover, the binder material plays an important role in getting significant behaviour of composite (*Hassan et al.* 2021). The metal oxide nanoparticle is widespread in various applications and owns better specific properties (Zadehnazari, 2023) reasons, and the metal oxide particle is taken (Hussain *et al.* 2022). The present research explores

the way various binders affect an entire system in several ways, including structural variations and variations in performance. It examines the relationship among MONPs and polymers in an array of settings, providing information into the material's variation, stability, and resulting properties through extensive examination and testing. Fig. 1 presents the various electrode preparation techniques.

Since electrode implementation features could influence the final efficiency of WO_3 , these have to be taken into consideration when evaluating the electrodes that are used for storing energy. A magnetic field must be present to start the storage of energy mechanism, and there must be good electrical contact between the material that acts as the backing board. The following is an overview of the most commonly used technique for making WO_3 electrodes.



Fig. 1: Flow process diagram for electrode preparation techniques

Metal mesh, copper or titanium foil, fluorine tin oxide (FTO) coated glass, and carbon-based substrates are commonly used for electrodes. The electrode structure can be created using one of two methods, as shown in Figure 1: either by coating a uniform WO3based solution onto the electrode's outer layer (for example, through drop casting or spin coating) or by directly producing the active ingredients onto the outermost portion of the electrode. Typically, an adhesive (such as Nafion, polyvinylidene fluoride or PVDF, or a substance called poly PTFE) and a material that conducts electricity (such as carbon black or acetone black) are mixed with various quantities of electrically charged material (such as WO₃ nanostructures) to generate a homogeneous slurry. A binder serves as a dispersion agent, improves adherence to the substrate, and binds the tiny structures together. The conducting material is used to enhance the electron conductivity of the electrically and biologically active material.

Additionally, a mixture of electrically charged substance, conductive material, and binder is mixed with various solvents such as deionized water, ethanol, and N-Methyl-2-pyrrolidone (NMP) to improve the slurry's uniformity. The conducting electrodes have been coated with a slurry of tungsten oxide nanorods that are carbon black and polyvinylidene fluoride, or PVDF, at an amount of 80%, 5%, and 15%, respectively, sprayed in the fall. The electrode was developed by dropping a solution of ethanol comprising porous lignin-derived charcoal (HPC)/WO₃, tiny structures, acetylene black, and Teflon at a ratio of 8:1:1 on an aluminium grid, placing a homogenous solution of WO₃/graphene nanocomposites that and PVDF dispersed within 2 ml of NMP on an aluminium sheet electrode. Drop casting onto an aluminium current collector a homogeneous slurry prepared by mixing WO_3 nanostructures, carbon black, and PVDF (70:20:10%) in a certain amount of NMP were used. A homogeneous slurry is prepared by mixing WO₃, carbon dioxide black, and PVDF (8:1:1) in the NMP and coating a carbon cloth material. The main problems of electrodes to be produced to the adherence of nanoparticles on the substrate and their durability, notwithstanding the efforts of scientists to determine the well-optimized uniform slurry content. Direct manufacturing of active substances on the substrate is used to create the electrodes, which solves this problem. There's an intimate connection between the way of manufacturing and the persistence of active quality. Fig. 1 shows the most prevalent kinds of synthesizing, including solvothermal and hydrothermal manufacturing, chemical bath deposition, and electrodeposition.

3. MATERIALS AND METHOD

Moreover, during the Multimodal Binder Optimization Characterization Modeling process, the scalability of polymer nanocomposite is studied with different parameters like curing time, magnification range and scalability ratios across diverse datasets considered. Based on this, the outcomes like performance analysis ratio were executed with M-MBOCM and SCB. During the evaluation, prototype testing was conducted and scale–up action was made with Characterization binders (SCB).

3.1 Performance Analysis

Comparing the Performance Analysis with M-MBOCM, as shown in Fig. 2, allows for an in-depth assessment of M-MBOCM's efficacy in optimizing binder selection for nanocomposite materials. M-MBOCM is a modern facilities instrument that can completely revamp the way scientists and engineers choose binders. The importance of M-MBOCM in tackling the difficulties of scaling up binder selection processes for industrial applications, as well as its efficiency and flexibility, are explored.

The efficiency of Multimodal Binder Optimization Characterization Modeling (M-MBOCM) is a giant step forward for the selection of binders for nanocomposite materials. M-MBOCM is an effective and forward-thinking tool for scientists and engineers due to its strengths in a number of important areas. When it comes to forecasting how metal oxide nanoparticles would behave in polymer nanocomposites, M-MBOCM has proved to be remarkably accurate. This facilitates a detailed comprehension of the interactions between various binders, the nanoparticles, and the polymer matrix. This precision is crucial for tailoring materials for specific uses, as it allows for the selection of binders that are guaranteed to produce the necessary material qualities (Otgonbayar et al. 2023; Chakrabarti et al. 2022). M-MBOCM has the advantage of being very efficient. It streamlines the procedure for choosing a binder, which cuts down the need for costly and time-consuming experimentation. Various binder alternatives and configurations can be rapidly evaluated, speeding up the overall development of nanocomposite materials. In fields where speed to market is paramount, this efficiency is essential. It's useful for many things, including batteries, bridges, and sensors.



Fig. 2: Performance analysis ratio (%) vs Number of datasets (M-MBOCM)

It is observed from Fig. 2 that the performance analysis ratio (%) results from manganese dioxide-based cathodes (M-BC), hybrid supercapacitors (HS), and nonenzymatic glucose sensors (NEGS) are related to advance M-MBOCM is recorded as maximum performance. According to this analysis, the binder action performance on the metal oxide nanoparticle-made composite is exposed to better value and progressively hiked by the increased numbers of datasheets. With this, the binder action of more than 60 numbers of datasets is recorded by more than 55 % of performance. However, the improved number of datasets may influence to hiked performance of polymer nanocomposite bound with metal oxide nanoparticles(Zadehnazari, 2023; Patil *et al.* 2022).

Fig. 3 expands on this comparison by contrasting Performance Analysis with SCB (Standard Computational Binders), providing insight into the relative efficacy of M-MBOCM in improving material characteristics and overall performance.



Fig. 3: Performance analysis ratio (%) vs Number of datasets (SCB)

Scientists can optimize the material qualities for a variety of uses by selecting binders that best suit each project's requirements. M-MBOCM helps the cause of sustainability because it takes into account the environmental impact of binder choice. It is in line with the increased focus on eco-friendly materials across sectors since it finds a happy medium between enhanced material performance and reduced environmental repercussions. Multimodal Binder Optimization Characterization Modeling (M-MBOCM) performance is distinguished by precision, efficiency, adaptability, and a focus on sustainability. This method of modelling allows scientists to make educated binder selections, which in turn leads to the creation of cutting-edge nanocomposite materials that are both technologically and industrially advanced and have a reduced ecological footprint. Therefore, M-MBOCM is a crucial resource in the search for sustainable and cutting-edge materials. However, the investigational analysis results of performance analysis ratio (%) from manganese dioxide-based cathodes (M-BC), hybrid supercapacitors (HS), and non-enzymatic glucose sensors (NEGS) are recorded better performance values and these values are related to SCM value found higher value of 96 % on 100 numbers of datasets. With the binder action, the performance of polymer nanocomposite is progressively hiked from 43 % to 96 % on the datasets from 0 to 100. More than 60 numbers of datasets illustrate a better performance analysis ratio (%). which indicates more than 55 %. The adhesive action and compatibility are the main roles of better binding action (Javed *et al.* 2023; Yadav *et al.*2023).

3.2 Scalability Analysis

M-MBOCM is contrasted with the Scalability Analysis to show how well it handles the varying scales and degrees of complexity in the binder selection process is highlighted in Fig. 4.



Fig. 4: Scalability Analysis ratio (%) vs Number of datasets (M-MBOCM)

Multimodal Optimization Binder Characterization Modeling (M-MBOCM) relies heavily on its scalability, which is a key factor in establishing the new tool's actual usefulness. The scalability of M-MBOCM is exemplified by the ease with which it may be transferred from the realm of basic research to that of mass production and widespread application. M-MBOCM's primary goal is to help researchers overcome growing difficulty of binder selection for the nanocomposite material creation. The ability to scale up the binder optimization process is crucial as more and more industries look to exploit the potential of these sophisticated materials for uses ranging from electronics to energy storage. M-MBOCM's computational nature is one of its main benefits when it comes to scalability. It takes advantage of high-performance computation to assess numerous binder combinations of interest to researchers speedily. Binder selection efforts may be scaled to manage larger datasets and more complicated material systems because of this computational efficiency. The flexibility of M-MBOCM is another factor in its scalability.

With the HS investigational analysis, results showed major variations related to a number of datasets due to unavoidable error action during the execution of analysis. The analysis results of the scalability analysis ratio (%) of M-BC and NEGS are recorded as better values and it is seen in Fig. 4. The M-MBOCM trends show the maximum scalability of binding action over the polymer nanocomposite, which results in the better energy performance (Yadav *et al.* 2023; Chandradass et al. 2023). Comparable to others, the M-MBOCM technique provides a dendritic enhancement in scalability performance, and 100 numbers of datasets spot 93 %.



Fig. 5: Scalability Analysis ratio (%) vs Number of datasets (SCB)

Fig.5 goes further by comparing Scalability Analysis to SCB, highlighting the scalability benefits of M-MBOCM for efficient and reliable nanocomposite material synthesis across industry and research applications. As the complexity of nanocomposite materials grows, this method will stay applicable and successful since it may be used with a wide range of metal oxide nanoparticles, polymer matrices, and binder ingredients. M-MBOCM may be automated and integrated with industrial processes, which adds to its scalability. Researchers can effectively implement M- MBOCM in real-world production settings, where consistency, efficiency, and dependability are of the utmost importance, by establishing streamlined workflows and automated procedures. M-MBOCM's scalability demonstrates that it is up to the task of meeting the difficulties associated with expanding binder choices during the creation of nanocomposite materials. Because of its computational efficiency, flexibility, and capacity for automation, it has the potential to propel innovation and growth across a wide range of technological and industrial fields, with the primary goal of capitalizing on the advantages of nanocomposite materials on an industrial scale.

The scalability analysis ratio (%) of HS indicates the lowest performance and recorded marginal enhancement in the scalability analysis ratio (%), which is lower than other results. More than 70 numbers of datasets, more than 40 %, are followed and the SCB results are recorded as better scalability value. However, the scalability analysis ratio (%) is progressively improved by the improved number of datasets. As a result of its high performance and its potential for large-scale production, M-MBOCM is an essential instrument for improving binder choice and accelerating the widespread use of advanced nanocomposite materials.

3.3. Relates to Applications

The characteristics of an ideal cathode are excellent electrochemical stability, resistance to the accumulation of discharge products, outstanding catalytic activity, quick CO_2 propagation, and rational structural design in Fig. 6.



Fig. 6: Schematic Illustrations of Catalytic Activity and Its Influencing Elements

Electrical carbon, binders, and catalysts are the primary elements of the cathode materials. Changes in

conductivity, porosity, catalytic function, and wetting may come from variations in both cathodic component

concentrations. Electrode material's particular surface area and cathode component ratio also play a crucial role. Discharge by-products that may settle on the electrode structure influence the total particular size and the energy density of $MeCO_2$ electrodes. The discharge product could disintegrate in the liquid electrolyte of a CO_2 battery if it is in a water-based solution. Discharge byproducts soluble in nonaqueous aprotic electrolytes are exceedingly unlikely to escape the cathode's pores. A cathode is utilized to hold the solid discharge result and block the flow channel for the carbon dioxide and solution gases. As shown in the image, the breakdown and dispersion of CO_2 in an electrolyte are aided by the porous nature of a highly appropriate surface that provides abundant chemical active sites with efficient mass-transfer passageways. As a result, most $MeCO_2$ cells use carbon with pores for their anodes. Soaking of electrolytes, solubility of CO_2 , and transfer of mass of CO_2 and electrolytes are all assisted by porous materials consisting of macropores, apertures, and pores. The storage capacity of $MeCO_2$ cells are enhanced by including meso- and macropores, which additionally offer adequate room for the deposit of solid products. But the electrochemical efficacy of $MeCO_2$ is impaired by the fact that tiny holes can efficiently transport pollutants, but can be easily obstructed by the emission of discharges products.

Intercalative pseudo capacitance is a relatively recent process for storing energy in pseudo capacitors Fig. 7.



Fig. 7: Diverse Energy Storage Systems and their Underlying Mechanisms

Electrochemical ions are stored in interactive pseudo capacitors by being inserted into conductive tunnels or layers of pore electrode materials. Although the diffusion of electrolyte ions (such as Li⁺) inside the crystalline structure of the electrode's substance controls the reaction dynamics in batteries, this is not applicable in intercalative pseudo-capacitance. This implies that the capacity is instead insensitive to variations in scanning rate, as the storage mechanism for intercalated ions is not followed by modifications in the structure of the substance of the electrode in Fig. 3. The incorporation of ions into layers of material is widely used in energy storage devices like batteries and capacitors that conduct electricity. However, few fundamental components contain ions that are somewhat bigger than lithium. Pseudocapacitive uses for acidic aqueous and nonaqueous electrolytes are possible due to the wide active surface made possible because of the rapid ion insertion characteristic of MXenes. In 2013, the first instance of MXene in a condenser electrode was reported. Ions from different solutions of salt have been discovered to be intercalated within MXene layers in this study, denoted in Fig. 8.



Fig. 8: The Processes Used to Create MXene SCs Interdigital

Further, the MXenes combine 2D conducting carbide layers with a predominantly hydroxyl-terminated aqueous surface. Therefore, MXene $(Ti_3C_2T_x)$ flake and $(Ti_3C_2T_x)$ Binder-free sheets were both explored and used as capacitive electrodes in this research. Their shows investigation that both exfoliated $(Ti_3C_2T_x)$ multilayers and MXene paper, consisting of many different $(Ti_3C_2T_x)$ layers, can intercalate various cations into water solutions. The way this occurs is moulded by the pH and the cation's composition. $(Ti_3C_2T_x)$ Significant intercalation capacitances were discovered by a comprehensive study of the chemical composition in these electrolyte solutions. The first study of the material in capacitance containing mono- and multivalent ions opens the way for additional research into the potential of the 2D family for use in electrolytic energy storage. For the synthesis of the ternary hetero, an HF solvent was employed in the previous study, whereas a blend of LiF and HCl was used as the wiping agent for another investigation. The scientists found no apparent shift in capacitance following 10,000 cycles at 10 A g1 for the LiF/HCl-etched Ti_3C_2 (MXene) clay. The capacitance as high as 380 F g1 or 1500 F cm³ was also achieved with hydrogel $Ti_3C_2T_x$ (MXene) electrodes in $3M H_2 SO_4$ electrolyte by employing transparent carbon current collectors; nevertheless, the energy storage of the MXene-based electrode failed to improve upon the earlier findings.

4. CONCLUSIONS

The performance of polymer nanocomposites is strongly influenced by the type of binders used, whether aqueous or nonaqueous. It is essential to highlight the significant impact of metal oxide nanoparticles on the performance of these materials in this comprehensive analysis. The complex structure of nanocomposite materials presents several challenges that need to be addressed, including achieving optimal nanoparticle dispersion, ensuring compatibility with binders, and addressing environmental concerns. The Multimodal Binder Optimization Characterization Modeling (M-MBOCM) is proposed as an effective method to comprehensively understand the intricate interactions among nanoparticles, polymer matrices, and binders. The performance analysis ratio, as revealed by both M-MBOCM and SCM analysis, stands at an impressive 95%. This research significantly advances our understanding and provides a valuable tool for optimizing binder choices through the application of this groundbreaking modelling strategy. These nanocomposites show tremendous potential for applications in high-capacity energy storage, lightweight structural materials, and cutting-edge smart sensors. Careful selection of binders has the power to enhance material quality, meet specific requirements, and minimize environmental impact. The meticulous simulation assessments carried out in this research validate the proposed approaches and provide deeper insights into the profound impact of a material's binder choice on its properties. Through the advanced methods of M-MBOCM and SCM, the scalability analysis ratio of binders and their effects on metal oxide nanoparticle of polymer nanocomposites overshadow those manganese dioxide-based cathodes (M-BC), hybrid supercapacitors (HS), and non-enzymatic glucose sensors (NEGS), with remarkable recorded percentages of 93% and 88% on M-MBOCM and SCM analyses

respectively. These findings not only confirm the potential of enhanced nanocomposite materials but also pave the way for their widespread application across diverse industries, offering innovative solutions to meet the ever-evolving demands in the fields of technology, energy, and materials science.

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CONFLICTS OF INTEREST

The authors declare that there is no conflict of interest.

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