SYNTHESIS, CHARACTERIZATION AND PROCESSING OF NEW MATERIALS FOR INNOVATIVE APPLICATIONS
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EDITORIAL

Machine learning in materials synthesis and characterization

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Machine learning (ML) is considered a promising tool in materials synthesis and characterization, and its innovative application in the near future because of its high compatibility with imaging, prediction, simulation, and natural language processing [1-4]. Depending on the intended application of the generated materials, operating conditions are often optimized during regular material synthesis and preparation [5]. In this context, ML models based on experimental data may be helpful to improve the synthesis procedures and their parameters in the event that simulations are successful. This necessitates the creation of novel data-driven techniques for identifying patterns across various length, time, and structure-property correlations. In terms of their characterization, analysis, and expansion of applications, these data-driven approaches exhibit significant promise in materials research [6,7]. ML models have recently demonstrated that a number of criteria related to the structure and processing of materials impact the characteristics and functionality of manufactured components, which in turn impacts the performance of the materials. ML can also be used to predict material properties and their classification based on different parameters [8-10].

Additionally, numerous studies have demonstrated the value of using ML-based algorithms to classify materials accurately based on various factors, including size, shape, and chemical and physical characteristics [11-13]. However, the lack of new knowledge and understanding resulting from the developed models is the main criticism of these methods in science.

The main reason for this is that more advanced applications of ML are frequently viewed as "black boxes." These computer-generated models are challenging for people to comprehend [14]. Additional restrictions, particularly for scientific models, include a limited number of parameters and conformity to physical principles. One of the major roles of data science is data collection and simulation, using accurate models to forecast material properties or to predict their classification and investigate their applications. Various models, including but not limited to cross-validation and careful selection, are useful methods to build accurate, simple, and efficient models [15,16]. Although ML approaches offer a wide range of intriguing possibilities for materials design, they also have several drawbacks and space for improvement. It is difficult to determine the accuracy, quality, and availability of the data and statistics used in ML because there are insufficient ground truth data, comparison metrics, or potentially irreproducible data [17]. The most recent developments and difficulties with applying ML in materials science were outlined by Choudhary et al. in their summary [18]. The authors of this review article discussed the evolution of computational approaches, the difficulties they encounter with normalization, ethics, and regulations, as well as issues with algorithm validation and interpretability, training-validation-test-related issues, and normalizing. The materials science community requires more technical research and laboratory procedures to create accurate and efficient artificial intelligence (AI) models to overcome its current obstacles and open up new possibilities for practical applications.

The use of Bayesian meta-learning algorithms to automatically enhance bulk crystallinity over numerous Joule heating reactions has been described as a practical use of ML models [19] to improve materials synthesis, operational conditions optimization, and achieve outstanding materials with desired properties.

Saad et al. noted that four alternative ML models were created in energy storage systems [20]. Compared to other models created for this purpose, the constructed artificial neural network (ANN) model produces exceptionally accurate prediction results, with a root-mean-square deviation (RMSE) of approximately 60.42. In addition, based on the findings of the work, the authors concluded that the combination of oxygen and graphene had the biggest impact on the ANN model.

In our most recent work, as shown in Figure 1, we created a brand-new artificial neural network based on the results of an electrochemical sensor for selective detection of catechol made of molecularly imprinted polymers and reduced graphene oxide (MIP/rGO@Fe3O4/GCE). The study proposed a solution to detect lower concentrations of the analyte that are lower than the limit of detection using an application of a new artificial neural network model [21].

Numerous studies have shown that ML imaging-based models can accurately discriminate between different materials based on their morphological traits. In a recent study, a very interesting model has been developed to investigate the structure and morphology of synthesized carbon nanotubes (CNTs) [22]. To establish mechanical properties, a mechanical compression simulation was employed. Deep learning (DL) neural networks were also created to forecast the class label for the CNTs generated images. These networks were validated and tested using FEM physics-simulation approaches. Another ML model is then used to forecast the physical stress of CNT forest physical and growth features [22,23].

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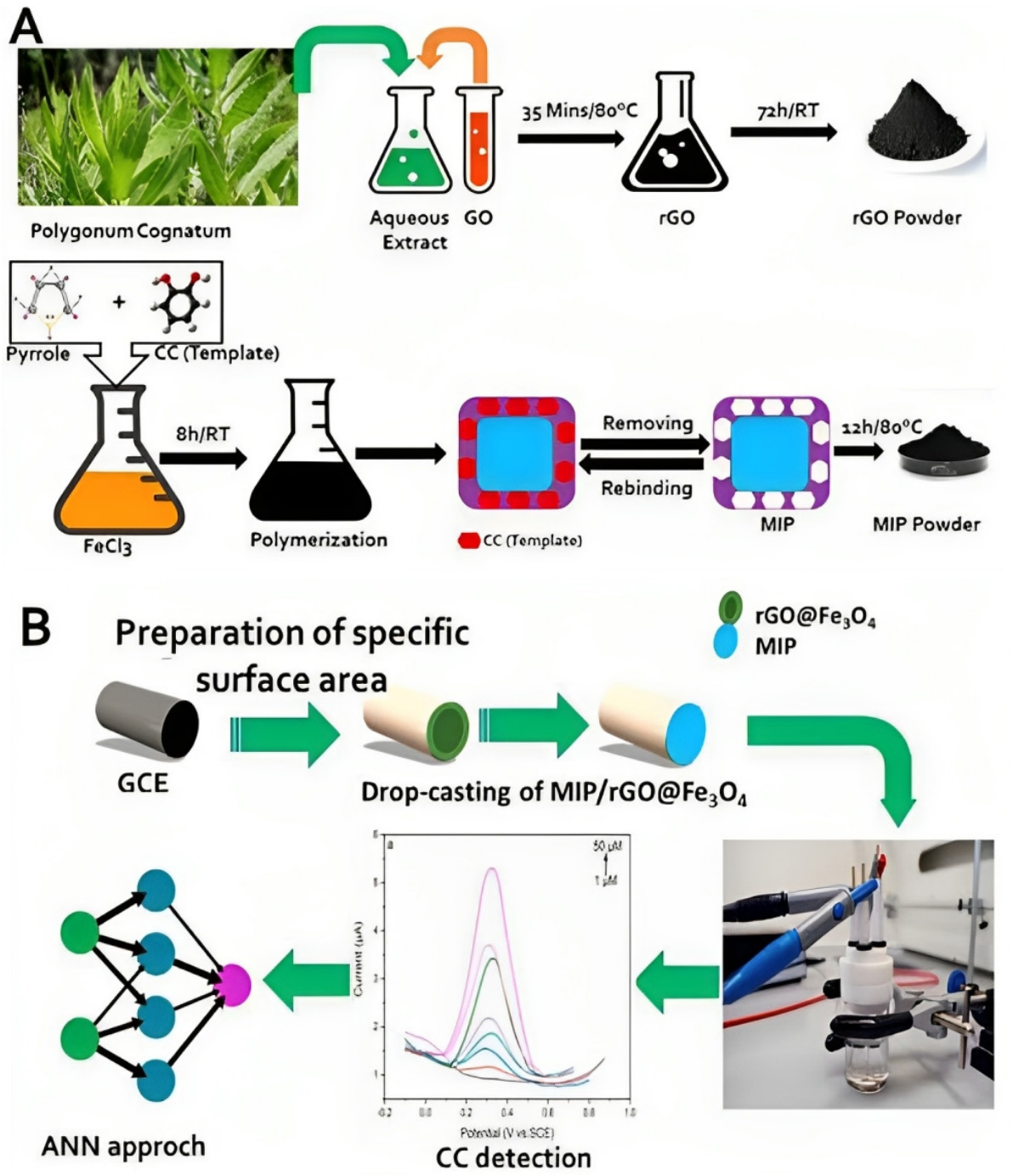

Figure 1. (A): Synthesis procedure of MIP and GO@Fe3O4 and (B): Catechol detection and artificial neural network preparation. Reproduced with permission from IOP [21].

In another study, Matos et al. presented a predictive multiscale model of the multiaxial strain-sensing response of conductive CNT-polymer composites. Detailed physically-based finite element (FE) models at the micron scale are used to produce training data for an artificial neural network; the latter is then used, at the macroscopic scale, to predict the electro-mechanical response of components of arbitrary shape subject to a non-uniform, multiaxial strain field, allowing savings in computational time of six orders of magnitude. We apply this methodology to explore the application of CNT-polymer composites to construct different types of sensors and damage detection [23].

In conclusion, ML applications in materials science have significantly contributed to understanding the interactions between materials, properties prediction, classification, and new materials development. However, different ML algorithms' prediction accuracy and efficiency vary for various metal-based nanomaterials challenges. It is crucial to evaluate recent developments in the application of ML approaches for challenges involving metal-based nanomaterials because of this and the high dimensionality and nonlinearity of the

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datasets that are now accessible. Future research is planned to help boost interest in this new and under-explored field of materials informatics and understand the applicability of various ML algorithms to various types of metal-based nanomaterials challenges.

ML approaches have the ability to change how the community views the link between experiment, simulation, and theory. The combination of ML, experiment, and simulation, when combined with automation (robotics), has the potential to construct integrated systems that optimize and unlock their applications in materials science. To summarize, ML-based methods in materials science are a rapidly growing subject. The problems ahead involve determining synthesis and characterization outputs, rates, and (internal) state distributions in a precise, quantitative, and thorough manner.

When combined with robotic platforms, ML can optimize reaction yields and conditions to control materials synthesis and acquire the desired attributes depending on the application. Appreciable improvements in turnover rates can be expected in the field of enzyme design for materials functionalization from coupling experiments with ML-based approaches. Recent advances in protein structure prediction will provide important insights for protein-lig interaction and recognition. Finally, for specific processes (e.g., methane oxidation), exploring whole reaction networks has only recently become practical. Exploration of materials synthesis, physical sciences, and chemistry will become feasible with enhanced, high-quality reference data.

Disclosure statement

No potential conflict of interest was reported by the author.

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