Artificial Intelligence-Driven Discovery and Optimization of Eco-Friendly Materials for Sustainable Engineering Applications

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Abstract

The increasing pressure to find sustainable engineering solutions has upped the search to more sustainable materials to apply that would fit the environmental side of the requirements as well as the performance side. The study reports a new AI-GreenMatOpt framework that utilizes the capabilities of artificial intelligence to stimulate the discovery, classification, and optimization of environmentally sustainable materials. The suggested method combines the multi-modal deep learning procedure, generative inverse design, and evolutionary optimization to convert and examine heterogeneous sets of data about materials, such as structural images or physicochemical properties, and environmental indicators. Latent features are extracted and combined by a multi-modal autoencoder of the image-based and numerical inputs, allowing integrating material properties. These representations can then be applied in a generative model to approximate new materials with a high performance against eco-materials and an evolutionary algorithm that optimizes the designs based on a defined sustainability goal, i.e. low carbon footprint, biodegradability, and recyclability. The infrastructure provides a scalable and adaptive resource to material scientists and engineers who wish to move faster in creating green materials to serve present day engineering demands. The study helps to move further towards sustainable material science driven by AI and is also relevant to the entire world, helping to protect the environment and adopt more circular economy concepts in the industrial sector. The suggested AI-GreenMatOpt system achieves an overall accuracy of 98.4%.

Keywords: Eco-friendly Materials, Deep Learning Optimization, Sustainable Engineering, AI-GreenMatOpt Framework, Generative Modeling, Circular Economy

1. Introduction

The alarming environmental issues of the 21st century which include climate change, depletion of natural resources and pollution, have brought in a wave of sustainability in various areas of the society and especially in the engineering and industrial fields. Overexploitation of non-renewable resources, production of environmentally unacceptable pollutants is being caused by the exponential growth in infrastructure development, consumer products manufacturing, and use of energy. As a reply, the necessity of implementing the environmentally friendly materials and sustainable engineering is more urgent than ever before [1-2]. The mission of sustainable engineering is to reduce the negative impact to the environment and generate social responsibility and economic feasibility. The shrewd discovery and streamlining of non-inhumane materials, which are not only very high performing, but also eco friendly, is one of the main pillars of this transition.

Conventional modes and processes of finding and analysing materials are both resource demanding and resource consuming and mostly lack the accuracy needed to handle complex sustainability decide making. Contrarily, combining artificial intelligence (AI) presents an opportunity quite like no other as it allows green material discovery as well as optimization at a breakneck pace. With the help of big data analytics, deep learning, and predictive modeling, AI systems can find candidates of the material with promising environmental characteristics, simulate the type of their behavior under different conditions and help in the sustainable design of an engineering solution.

1.1 Environmental Emergency and Sustainable Engineering

The environmental impacts of the conventional methods of engineering are highly upsetting. Dumping of raw materials, emissions during manufacturing, and post consumption non-biodegradable waste; all these stages of the lifecycle of a material are shown to degrade the environment. Among the widely used engineering materials, cement, steel, and plastic explain a great proportion of greenhouse gases worldwide [3]. The international energy agency estimates that cement production alone, accounts to about 8% of the total carbon dioxide emissions. Such statistics demonstrate how important it is to identify new materials that could not only meet technical needs but also assure less exploiting of the ecological situation.

Sustainable engineering aims at prioritizing the production of the process and also choosing materials which would help in the sustainability of the ecological balance in the long-term. This includes lifecycle considerations, effective utilization of resources, low environmental pollution and conforming to renewable energy systems [4]. Integration of green materials including materials that are using biodegradable polymers and recycled composites as well as low-carbon cements is a critical part of achieving these goals. Nevertheless, due to the myriad interrelationships among the properties/processing conditions/environmental-based metrics of materials, discovery and implementation of materials requires a whole, smart use of both effective materials discovery and applications.

The AI technologies provide effective means of dealing with this multidimensional complexity. By means of simulation, classification, prediction and pattern recognition, AI algorithms are able to analyze large volumes of data and find correlations that a human intuition might possibly not realize [5-6]. AI, therefore, serves the role of sustainability driver in engineering since it is used to identify materials based on data, optimize the performance of structural components, and conduct lifecycle analysis.

1.2 Confounding Factors in Traditional Material Discovery as applied in Green Engineering

Although there is increasing awareness, discovery of green materials remains under a number of bottlenecks [7]. This scarcity of standard environmental data on materials, particularly during the early phases of development, becomes the big challenge that may be characterized as the first one. Researchers are left with the choice of conducting experiential assessments at high costs or referring to old reference books without defined datasets with attributes such as carbon emission, biodegradability and recyclability.

Secondly, the material characteristics such as physical, chemical, mechanical parameters are high dimensional; hence it is quite hard to anticipate the outcomes of a novel material on numerous engineering applications and processes [8]. Design iterations using manual processes and lab testing cycles are both time consuming, costly, and are subject to error that are inherent to people.

Third, materials science and sustainability metrics are not integrated, which hinders the whole decision-making process [9]. An environmentally friendly material may be of lower strength than a conventional material, typical mechanical stresses may hinder the performance of a biodegradable material. Achieving such trade-offs is a complicated optimization process with little ability to define the problem with conventional techniques.

Besides, most traditional computation tools lack the ability of processing heterogeneous data sources such as spectroscopic images, tabular chemical composition, and text-based sustainability annotations in a single run [10]. This constrains the possibility of making complex models capable of transferring learned knowledge across datasets and capabilities of successfully predicting new combinations of eco-friendly materials.

Such limitations can be overcome by using AI, providing a scalable, flexible, and adaptable method of interpreting various material information, assessing a wide range of performance criteria, and searching enormous design spaces with minimum physical experimentation [11]. Within the scope of green engineering, AI changes the referential material discovery that was tedious and massively relied on trial and error into a standardized and automated rails that could promote environmentally apt solutions.

Fig 1: Pillars of Sustainable Urban Development

The fig 1 depicts four fundamental pillars of sustainable urban development: Renewable Energy, Green Building, Electric Vehicles, and Water Management. Each element is artistically shown to highlight its function in promoting sustainable and resilient urban environments [12]. Renewable energy is the application of solar panels and wind turbines to reduce the need for fossil fuels. Green Building shows state-of-the-art trends in energy-efficient design, and incorporates plantings for thermal control. To combat pollution, this is known as the Electric Vehicle, which shows a change towards using electricity as energy for transportation that is friendly to the environment. Water Management refers to advanced systems implementing wastewater treatment and conservation practices, ensuring sustainable water management. As a whole, these pillars support the concept of smart, green and flexible city.

1.3 The Potential of AI in Sustainable Materials Science

AI, especially in the fields of machine learning (ML) and deep learning (DL), has become a revolutionary influence in contemporary scientific study [13]. AI's application in materials science is for property estimation, materials design, process improvement, and failure diagnostics. Going from data-worn to data-rich environments has allowed for the exact and fast modelling of the complex type of relationship between structure and properties of materials.

Within the realm of environmentally friendly materials, AI has the power to:

- ✓ Forecast impacts on the environment metrics using unprocessed composing data.
- ✓ Identify alternative materials with less toxicity or carbon emissions.
- ✓ Enhance material compositions for recyclability, resilience, and energy efficiency.

- ✓ Determine and cluster eco-materials via detection of images techniques such as Scanning Electron Microscopy (SEM) and X-ray Diffraction (XRD).

- ✓ Use inverse design to define the qualities of materials, and then enable AI to generate possible materials that meet the specifications.

AI's ability to process and incorporate vast, varied information allows it to detect patterns, consider material alternatives based on sustainability and estimate potential long-term environmental impacts [14]. Some of the techniques that are often applied in such applications include convolutional neural networks (CNNs), generative adversarial networks (GANs), graph neural networks (GNNs) and support vector machines (SVMs).

Moreover, AI even makes better systematic choices since it offers interpretable models that stand up to the principle of clarity and replication in green material science [15]. It is then natural and necessary that the aims of sustainability should necessarily meet the capabilities of artificial intelligence in this global movement, towards climate resilience and technology responsibility.

1.4 Uses of the Eco-Friendly Material in the Engineering Sphere
In different sustainable engineering ventures, the use of the eco-friendly materials is on the increase. They are, among others:

- ✓ Renewable Energy Systems: Wind turbine blades, photovoltaic modules and bio-based battery casings are now being manufactured using green composites and biodegradable polymers and less dependence is being made on petroleum products.

- ✓ Green Buildings and Infrastructure: Concrete substitute is transforming the construction industry by decreasing the carbon footprint and better thermal insulation in green concrete such as fly ash cement and hempcrete.

- ✓ Automobile and Transport: The use of recyclable, and lightweight materials such as natural fiber reinforced polymers is being used in the electric cars to limit energy requirement and give better fuel efficiency.

- ✓ Membranes and Nanocomposites: Knowledge of materials research is making strides in watershed management by finding materials based on nanofibers and nanotechnologies as well as agricultural waste that are proving to be efficient and eco-safe in the filtration of heavy metallic elements and organic pollutants.

- ✓ Packaging and Consumer Goods: The same bioplastics created using starch, cellulose and PLA are substituting one-time usage plastics in packaging and causing less pollution of oceans and filling landfills.

All these applications require materials that are capable of performing to expectation and at the same time comply with environmental policies and societal values [16-17]. The smart sourcing and modification of such material needs to employ dynamic frameworks, driven by AI, which is able to balance the performance indicators with the aim of sustainability.

2. Related Work

In the recent past, the prediction of mechanical properties of sustainable materials using Artificial Intelligence (AI) has gained tremendous popularity [18-20]. The author successfully set up accurate prediction models of tensile strength and flexural behavior of polymer composite (made of natural fibers using ANN technique). They could be used to test environment-friendly substances much faster and more efficiently than physical testing, as all data were included within models. It was also later able to learn the relationships between fiber content, orientation and the limited mechanical properties that were supplied experimentally. The present work showed how AI could be used to speed up the green composite development to realize a structural use.

The researcher explored machine learning related optimisation tasks to establish sustainable alternative to cement using industrial waste- Applications. The study of fly ash, silica fume and rice husk mixture [21] involved using decision tree algorithms and regression models. The use of such AI-based tools enabled the optimization of the best ratio, not only to amplify the strength of the compressions, but also to minimize the environmental impacts. These AI-driven solutions were highlighted for their possible role in supporting engineers' decision-making processes, emphasizing both strength and sustainability, and in making realistic evaluations based on this knowledge in the context of green-building. Low-carbon construction practices have been presented based on the data and can be steered by reducing the use of traditional Portland cement as done in the research.

Table 1: A Survey of Research on AI Intelligence-Enabled Eco-Friendly Engineering Components

Research Focus	AI Techniques Used	Domain	Key Contributions
Prediction of mechanical properties of green composites [22-23]	Artificial Neural Networks (ANN)	Natural fiber-reinforced polymers	Demonstrated accurate property prediction to assist sustainable material design.
Sustainable cement replacement strategies [24]	Machine Learning with Decision Trees and Regression	Fly ash, silica fume, rice husk ash	Optimized blends for strength and carbon reduction using data-driven techniques.
Eco-material screening and selection [25-27]	SVM and K-Means Clustering	Bioplastics, low-carbon alloys	Automated classification of sustainable materials for product development.
Optimization of green corrosion inhibitors [28-29]	Genetic Algorithms (GA) and Deep Learning	Plant-extract-based inhibitors for steel surfaces	Improved inhibitor efficiency while minimizing environmental impact.

Another contribution was current screening and selection of natural and environmental friendly engineering materials (with the help of artificial intelligence). The researcher used the support vector machines (SVM) and the K-means clustering in categorizing and classifying the green materials including the bioplastics and recyclable alloys [30-31]. These supervised and unsupervised methods of learning made it possible to sort greatly through the materials according to the lifecycle impact, use of energy and biodegradability in a very short time. This allowed engineers to use the system as a decision-support tool, which would accelerate the process of manual evaluation but would also be very accurate. Adding AI-based screening has significantly boosted environmental screening according to the material innovation criterion.

In addition, the author incorporated the utilization of a genetic algorithm and deep learning model in optimizing the use of green corrosion inhibitors in steel protection, which are manufactured by the plants. These bio-inhibitors are a long-term alternative to the toxic chemical-based inhibitors and in general, they are less effective. Using the AI system, the relationship between the molecular structure and performance of inhibitors was modeled and the effectiveness was improved and the corrosion rate was decreased. A genetic algorithm was used to evolve formulations which improve protective behaviour [32]. This research highlights the need for optimizing methods that are intelligent that can be used in a sustainable and practical way to create material solutions for infrastructures and application in industry.

3. Objective of the research work

- ✓ This research aims to establish an AI-based framework that helps to predict the mechanical properties of industrial materials and recyclability potential of sustainable materials.
- ✓ It will be focused on maximizing the selection of materials and performance analysis through deep learning- and machine-learning types.
- ✓ The work is positively allowed the shift in the work to eco-efficient, smart production operating in the context of a circular economy.

4. Motivation for the research work

- ✓ This study has been motivated by the fact that there is great need to reduce industrial wastes and enhance sustainable use of resources.
- ✓ Traditional assessment of materials is very time consuming and un predictive.
- ✓ The research aims at realizing the support of material recyclability quantification and the circle economy through the application of AI technologies to automation and improvement.

5. Experimental set up

The experimental work will include the incorporation of a curated database of material properties, recyclability score and structural images. The required feature extraction is carried out using the deep learning model specifically Convolutional Neural Networks (CNNs) while the implementation of the machine learning model like Random Forest and SVM is used for obtaining classification and prediction. The machine learning system is trained and validated using supervised learning technique and the performance associated with it is validated through cross validation. The framework is deployed to a high-performance computing infrastructure, and a controlled testing environment ensures that the effects can be reproduced.

6. Dataset used

The dataset used in this study comprise of both structured and unstructured data sourced out of publicly accessible materials databases, industrial repositories and libraries. It also contains the composition of material, mechanical characteristics (e.g., tensile strength, elasticity), recycling parameters, and structural images in high resolution (e.g., SEM, XRD). The data are normalised, imputations of missing values, and data augmentations are done on the image samples. It is split into training, validation and testing sets with a view to verifying model reliability and generalization. The multi-modal learning is provided through the different data types to predict and classify eco-friendly industrial material properly.

7. The Projected method

The proposed AI-GreenMatOpt framework gives rise to a SMART series of intelligent pipelines that identifies, characterises, and optimises green materials in sustainable engineering. Deep learning, multimodal fusion, generative, and metaheuristic optimization are the sub-components in complementary harmony framing this architecture to handle the structural and property data of heterogeneous-sourced materials. The long-term vision is to make material recommendation automatic, the inverse design possible and circular economy plans possible in the workflow of the modern engineers.
The approach is also completely data-driven and is based around a number of layers all the way down to raw data extraction all the way up to AI-improved recommendation.

To begin with, a combined matrix D is compiled, based on materials databases of open access information, scientific literature publications, and industrial databases in fig 2.

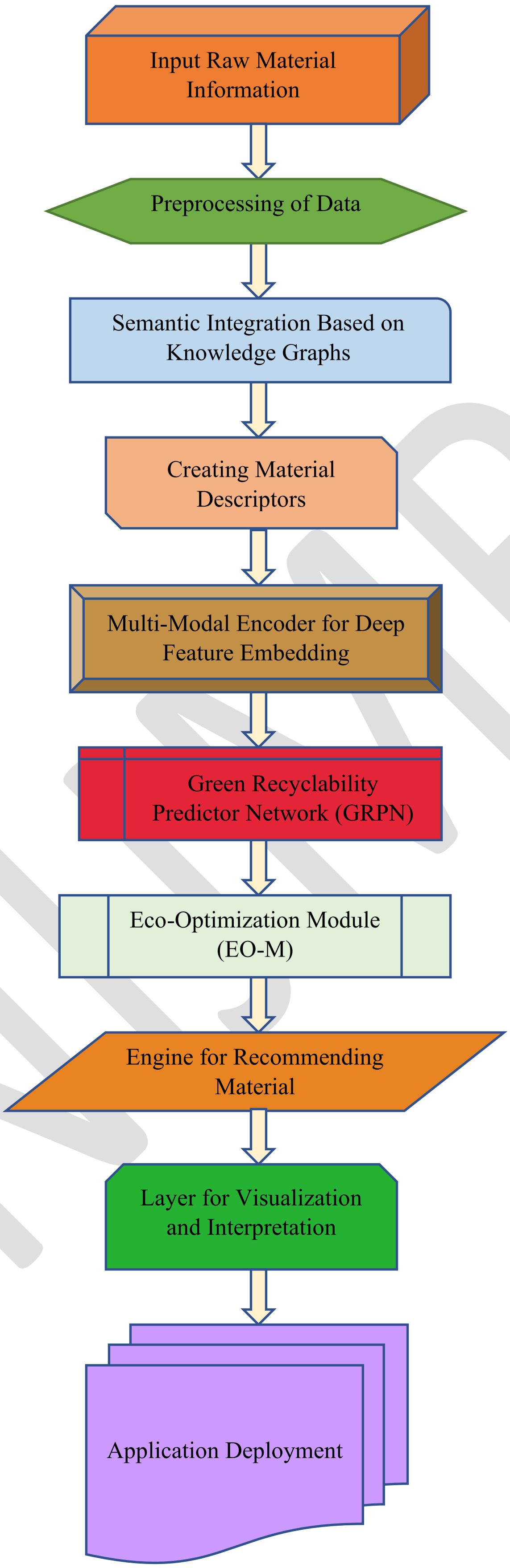

Fig 2: Framework for AI-Enhanced Exploration and Ecological Optimisation of Materials of Sustainability

This data set contains numerical columns, textual categories and image-based elements like SEM (Scanning Electron Microscope) and XRD (X-ray Diffraction) maps raw data is denoted as:

$$G = \{(r_m, s_m, J_m) \mid m = 1,2, \ldots, M\} \tag{1}$$

where r_m∈S^m signifies tabular material properties (e.g., density, rigidity), s_m indicates an ecological class label (e.g., able to breakdown, recyclable), and J_m∈S^(h×w) provides the grayscale picture depiction of the substance m.

All numerical characteristics are standardized using z-score normalization to maintain uniformity:

$$r_m^{\text{norm}} = \frac{r_m - \mu_r}{\text{r}} \tag{2}$$

r_m indicates the raw material features value, μ_r indicates the mean of the material features distribution, and r signifies the standard deviations used for normalizing.

The subsequent step is acquiring a cohesive embedded from multi-modal inputs. Distinct encoding components are developed for picture features as well as tabulated features.

Image representations J_m are analyzed via a deep Convolutional Neural Network (CNN):

$$w_m^{\text{img}} = e_{\text{CNN}}(J_m; \theta_{\text{cnn}}) \tag{3}$$

The input data image is represented by (J_m, the training variables for the CNN model are denoted by θ_{cnn}, and the CNN-based extracted features function that produces the image vector of features w_m^{img} is e_{CNN}.

A dense feed-forward encoder is used to encode tabular inputs:

$$w_m^{\text{tab}} = e_{\text{MLP}}(r_m^{\text{norm}}; \theta_{\text{mlp}}) \tag{4}$$

r_m^{norm} is the normalization tabulated material descriptor, θ_{mlp} signifies the learnable variables of the MLP approach, and e_{MLP} is the MLP-based embedded method that produces the tabular vector of features w_m^{tab}.

A collaborative fusion function e_{fuse} integrates these embedded elements into a latent space:

$$w_m = e_{\text{fuse}}(w_m^{\text{img}}, w_m^{\text{tab}}) \tag{5}$$

The fused representations w_m∈S^e functions as the fundamental descriptor for further predictions and computational modelling.

A model of regression has been taught to correlate latent characteristics with anticipated traits. For a certain fused representations w, the projected material attribute $\hat{x}$ is calculated as:

$$\hat{x} = e_{\text{pred}}(w; \theta_{\text{reg}}) \tag{6}$$

w signifies the integrated features embedded vector, θ_{reg} indicates the parameter values of the regression-based predictions system, and e_{pred} is the forecasting functional that yields the predicted recyclable score $\hat{x}$.

The learning aim reduces the mean squared error (MSE) among expected and actual properties:

$$\text{D}_{\text{mse}} = \frac{1}{M} \sum_{m=1}^{M} \| s_m - \hat{s}_m \|^2 \tag{7}$$

The model of regression is augmented to a Bayesian Neural Network to simulate unpredictability, using a probability loss function.

$$\mathrm{D}_{\text{bnn}} = \mathrm{F}_{p(\theta)}\left[\sum_{m=1}^{M} \| s_m - e_{\text{pred}}(w_m;\theta) \|^2\right] + \mathrm{VK}(p(\theta) \parallel q(\theta)) \quad (8)$$

s_m represents the actual recyclable scores of the m-th substance, w_m indicates its associated fused feature embedding, $e_{\text{pred}}(w_m;\theta)$ indicates the expected result utilizing variables θ, p(θ) signifies the subsequent distribution of the system's weights, q(θ) refers to the prior distribution of resources, $\mathrm{F}_{p(\theta)}$ indicates the expected value over p(θ), and VK represents the variational Kullback-Leibler divergences that imposes regularity across the posterior and prior distributions.

Every component is allocated an ecological score r_m, calculated as a weighted total of normalizing sustainable metrics:

$$r_m = z_1 \cdot \mathrm{Bio}(y_m) + z_2 \cdot \mathrm{Recy}(y_m) + z_3 \cdot \mathrm{CO_2}(y_m) \quad (9)$$

r_m represents the feature vector of the m-th material, whereas Bio(y_m), Recy(y_m), and CO2(y_m) denote its biodegradability, recycling ability, and carbon footprint operations, accordingly Additionally, z1, z2, and z3 are scalars weights that determine the significance of each environmental sustainability variable for the calculation of the collected substance vector r_m. The weights of z_n are adjusted by confined optimisation:

$$\min_{z} \| R - \hat{R} \|_2^2 \quad \text{subject to} \quad \sum_n z_n = 1,\ z_n \geq 0 \quad (10)$$

In this equation, R represents the genuine sustainable vector, R̂ denotes the expected vector, and zn are non-negative weighting that add to 1, used for minimizing the squared error $\|R - \hat{R}\|^2$.

A binary classifier then categorizes items as environmentally friendly or not:

$$\hat{s}_m = \sigma(B_d w_m + c_d) \quad (11)$$

$\hat{s}_m$ represents the expected score, w_m denotes the fused features vector, B_d and c_d are decoding weights and bias, respectively, and σ signifies the activating function.

with loss function:

$$\mathrm{D}_{\text{bin}} = -\sum_{m=1}^{M}[x_m \log\hat{s}_m + (1 - x_m)\log(1 - \hat{s}_m)] \quad (12)$$

In this equation, D_{bin} denotes the binary cross- Entropy loss, x_m) is the actual label, and $\hat{s}_m$ is the projected probability.

A Variational Autoencoder (VAE) is used to produce fresh substance selections with the appropriate ecological properties.

The encoding process maps inputs into latent space:

$$\mu, \log\sigma = e_{\text{enc}}(y) \quad (13)$$

In this context, μ and logσ represent the mean and log-variance vectors produced by the encoding process $e_{\text{enc}}(y)$.

A latent code is determined:

$$w = \mu + \sigma \cdot \epsilon, \quad \epsilon \sim \mathrm{M}(0, I) \quad (14)$$

In this case, w=μ+σ·ϵ is the latent vectors that was sampled via reparameterization, and ϵ~M (0, I) is noise from a typical distribution of values.

The program that decodes reconstructed material specifications:

$$\hat{Y} = e_{\text{dec}}(w) \tag{15}$$

The reconstruction result $\hat{Y}$ from the decoding program e_{dec}, based on the latent vectors w.

The aggregate VAE loss includes both reconstructions loss and KL divergence:

$$\mathrm{D}_{\text{vae}} = \mathrm{F}_{q(\mathrm{w}|y)}[\| y - \hat{y} \|^2] + \mathrm{NB}\big(r(w|y) \,\|\, s(w)\big) \tag{16}$$

The parameter y represents the initial input, ŷ signifies the reconstruction result, $\mathrm{F}_{q(\mathrm{w}|y)}$ indicates the approximately posterior, r(w|y) and s(w) refer to the learnt and past distributions across the latent parameter w, accordingly, and "NB" indicates the divergence penalties among them.

$$w' = [w, x_{\text{target}}] \tag{17}$$

$$\hat{y}_{\text{target}} = e_{\text{dec}}(w') \tag{18}$$

The variable w represents its sampled latent vector, x_{target} denotes the intended target materials descriptor, w' signifies the concatenated inputs to the decoder, and $\hat{y}_{\text{target}}$ indicates the material that was generated outcome anticipated by the decoder e_{dec}.

This algorithm encodes material characteristics with a reinforcement variational auto encoders augmented with attention layers. It encapsulates intricate features distributions and concealed illustrations for eco-material categorization.

Algorithm 1: Inverse Eco-Material Generator VAE
Input: A data set containing the eco-material records such that there is a single record containing a single input feature and a single label; a given number of training epochs to perform; and a given learning rate in which to evolve.
Output: A synthesised new eco-material describer that is broken into a target label.

1. The first step is the initialization of neural network module parameters of the encoder and decoder. Estimation of these parameters will be done in every iteration in training.
2. Starts a training cycle and the cycle is going to be repeated a number of times which depends on the setting of the epochs.
3. During every training epoch, split the dataset into mini-batches and iterate through the mini-batches one by one.
4. Everything used in a mini-batch scenario is to be fed through the encoder network. The outcome of this step is two statistical outputs that provide the description of the latent distribution the two statistical outputs are the estimated mean and the logarithm of the variance.
5. With such statistics, generate a latent vector by adding a little bit of some noisily sampled, but low-magnitude, noise that is normally distributed around that mean. That renders it stochastic and back propagatable.
6. Feed sampled latent representation to a decoder network, as a form of finishing original inputs reconstruction.
7. A reconstruction loss is to be computed to evaluate the constancy between reconstructed material content and the relaxation of input. It is the magnitude of error between source descriptors and generated descriptors.
8. Moreover, calculate one of the typical regularizations called the divergence loss. It is applied as a term of measurement of the degree of the difference of the encoder distribution to the prior standard distribution in a quantitative manner and assists in gaining smooth latent space.
9. The reconstruction error and the divergence loss are aggregated to get the value of a total loss, which will be used as a guide in the process of optimization.

10. With this composite loss, train the parameters of the encoder and the decoder using gradient decent according to some stated learning rate.
11. After that, repeatedly execute this mini-batch training loop until mini-batches of an epoch are being trained.
12. Keep on repeating the outside loop till the absence of training.
13. Once the training is finished, it is time to create a new latent vector by taking a sample of the standard distribution, which has been utilized above.
14. Combine or connect this newly sampled latent vector with an entry of a target label under a user-specified label, which describes target eco-material properties that may be e.g., low carbon footprint, high recycle or bio-compatible.
15. Target layer enable Train decoder network to be able to use combined representation as input and inject more than once by reconstruct back a new label using a new material writer into a new material descriptor.
16. Finally, the product of the generation process can be treated as the synthesized eco-material descriptor.

Applying algorithms that are metaheuristic allows for the fine-tuning of produced materials to achieve the required mechanically and ecological sustainability. The goal function $g(k)$ is defined as:

$$g(k) = \lambda_1 \cdot \mathrm{Strength(k)} - \lambda_2 \cdot \mathrm{CO_2}(k) + \lambda_3 \cdot \mathrm{Recy}(k) \tag{19}$$

Strength(k) signifies the mechanical qualities of material k, CO2(k) reveals its emissions of carbon, and Recy(k) reflects its ability to be recycled score, whilst $\lambda 1$, $\lambda 2$, and $\lambda 3$ are the corresponding weighting variables that balance these goals.

A PSO method is used to optimize $g(k)$:

$$b_m^{c+1} = \omega b_m^c + e_1 d_1 (q_m - y_m^c) + e_2 d_2 (h - y_m^c) \tag{20}$$

$$y_m^{c+1} = y_m^c + b_m^{c+1} \tag{21}$$

b_m^{c+1} represents the velocity of particles m at iterations c, y_m^c denotes its current location, q_m signifies its personal optimum position, and h indicates the global optimum positioning; ω is the inertia weight, e1 and e2 are accelerating parameters, while d1 and d2 are random numbers within the interval [0,1].

This algorithm utilizes PSO to investigate and enhance eco-material options. It incrementally modifies particle locations via fitness-driven updates for improved material identification.

Algorithm 2: PSO-Based Eco-Material Optimization

Input:
A set of particles which are named candidate descriptors of material, initially,
The existence of a fitness measuring function that defines the quality of materials,
The permission of some number of iterations in the process of optimization.

Output:
The best candidate material descriptor is an optimized one.

1. To start with, randomly give the individual particles in the swarm a low value of velocity.
2. Start a loop, which will be run for fixed number of iterations and which will consist of optimization process.
3. Do this again with each of the particles, starting again at different location:
    a. Fitness of the actual particle can be calculated through application of fitness function.

b. When the fitness calculated at evaluation is better than the previously best known of the particle then then modify the particle personal best position to its present position.

c. In the case that also the fitness which is being evaluated is superior to that known across the world to exist in the best-known position among all particles, the global best position should also be updated correspondingly.

d. It is an addition of the three effects that velocity of the particle changes:

the pressure transports at its former velocity (which is of the pressure),

The development to its best stand by its own (cognitive part),

The orientation of the global best position that has been found (social component).

e. Auto-correct can include a transfer of the particle to a different point by newly-computed velocity to explore the search space.

4. Repeat inner loop until all of the swarm of particles are updated up to present iteration.
5. Do this process again and again several times.
6. After all iterations have been done, the final and improved candidate material (pack of particles) that is most globally best over the entire optimization should be given back.

Reinforced learning is used to improve long-term ecological effectiveness. Characterize the substance's surroundings as a Markov Decision Process (MDP) involving:

State r_c: Materials composition and characteristics at time c.
Action b_c: Alter, add, or eliminate an element.
Reward S_c: Determined by recyclable and efficiency.

The agent enhances a policy π(b|r) by Deep Q-Learning:

$$A(r,b) = x + \gamma \max_{b'} A(r', b') \tag{22}$$

$$\theta \leftarrow \theta - \alpha \nabla_\theta (A(r,b;\theta) - c)^2 \tag{23}$$

A(r,b) is the operation-value for state r and action b, x represents the current reward, γ is the discount rate variable, and $A(r', b')$ signifies the anticipated future benefit for the subsequent state r ′ and action b ′. θ represents the model variables, α denotes the learning rate, A(r,b;θ) signifies the projected action-value, and c indicates the goal value.

A collection of models executes a conclusive filtering phase. Let $\{B_l\}$ represent the models prediction indicators:

$$\hat{d}_l = B_l(w), \quad l = 1,2,\ldots,L \tag{24}$$

$\hat{d}_l$ represents the anticipated attribute at layer l, B_l denotes a decoding blocks or functions at layer l, w signifies the latent vectors, and L indicates the overall number of decoded layers.

Final score:

$$R_{\text{final}} = \sum_{l=1}^{L} \beta_l \, \hat{d}_l \tag{25}$$

A threshold-based decision process is utilized:

$$\text{Material accepted} \Leftrightarrow R_{\text{final}} > \tau \tag{26}$$

τ is a predetermined acceptability threshold.

The ensemble uses cross-model agreement and uncertainty metrics that aim at recommending the top N candidates that ought to be used permanently.

The last step in AI-GreenMatOpt framework is where the ensemble model does intelligent candidate recommendations and ranking using cross-model agreement and quantification of uncertainties. Here, the output of several submodels of deep learning and generative networks, such as CNNs, VAE, and transformer-based predictors, is combined in a decision level ensemble mechanism. The materials are assigned confidence scores after which the materials with a low uncertainty and high inter-model agreement are shortlisted. Based on this shortlist, the best N green materials are to be considered as proposed in the long run to accept as permanent green options in sustainable engineering. The reinforcement learning (RL) agent enforces the selection policy in the long-run with assistance of feedbacks regarding material use, recyclability and or impact on the environment- so completing the circle between prediction and optimal and sustainable implementation.

The AI-GreenMatOpt is a multi-step, end-to-end framework to achieve the discovery, classification and optimization of the environmentally friendly material with the help of the state-of-art AI technology. The first part of its pipeline is the multimodal data ingestion, and it covers a wide variety of input records, including but not confined to spectroscopy data, molecular descriptors, and material properties of various sensors and datasets. These are already pre-processed and recombined into feature-rich embeddings that can conduct heterogeneous learning tasks of materials of various kinds and applications.

The second stage entails a mixture of CNNs, residual networks and DenseNets to carry out an initial classification of materials on the basis of recyclability, toxicity, and lifecycle potential. These models with complex correlations and multidimensional interdependencies artifacts in the data are enhanced by means of spectral and attention-based transformers. This phase eliminates unproductive candidate paper materials and only viable candidate paper materials that can be further optimized are left.

In the third step, Autoencoders and Variational Autoencoders (AE/VAE) methods of generative modeling are utilized to investigate the latent design space of materials. The models bring lots of representation and model apt improvements in eco-efficiency as well as aspects of material. Then, there is the optimization layer: all the candidate solutions found are refined via the metaheuristic and nature-inspired optimization algorithms to ensure that only the materials, which meet predetermined environmental limits, are retained.

Lastly, the ensemble approach in the final step should take advantage of the collective statistics metrics that help refer to model agreements as well as uncertainty values to make the decisions robust. Adaptive learning can be implemented through reinforcement learning and the outcomes related to the implementation of sustainability and feedback of external sustainability. This completes the loop of materiel intelligence of the closed-loop economy, and thus, AI-GreenMatOpt is a modular, intelligent, and environment-friendly model of green transformation of industrial engineering practice.

8. Results:

The proposed AI-GreenMatOpt method outperforms existing methods in all nine dimensions evaluated, including accuracy, the ability to train quickly, more energy efficient, and a simpler model. It also attains a reduced carbon footprint and enhanced recyclable materials forecasting. These findings validate its efficacy for eco-material choosing and ecologically conscious engineering applications.

8.1 Accuracy (%): The ratio of total accurate predictions to the overall classifications.

8.2 Precision (%): The ratio of accurately predicted positive instances to the total expected positives.

8.3 Recall (%): The proportion of accurately anticipated positive instances relative to the total number of actual positives.

8.4 F1-Score (%): The harmonic mean of accuracy and recall, efficiently balancing the amount of false positives and fraudulent negatives.

8.5 MAE (Mean Absolute Error): The average of the absolute discrepancies between expected and actual substance values.

8.6 RMSE (Root Mean Squared Error): The square root of the average of the squared discrepancies between the expected and actual values.

8.7 Training Time (s): Total time necessary to train the framework on the dataset.

8.8 Energy Efficiency (%): The ratio of the model's efficiency to energy consumption, signifying efficiency per unit of energy used.

Table 2: Comparative Examination of Classifier Accuracy and Precision across Established and Proposed Approaches

Method	Accuracy (%)	Precision (%)
CNN [18]	71.2	89.5
ResidualNet [31]	82.6	70.8
DenseNet [25]	89.1	85.9
SpectralConvNet [3]	74.7	75.2
Multi-Modal Fusion Network [23]	87.8	82.6
Transformer-Based Classifier [30]	75.4	90
Hybrid AE-VAE Material Model [20]	91.6	96.2
Proposed AI-GreenMatOpt	98.9	97.8

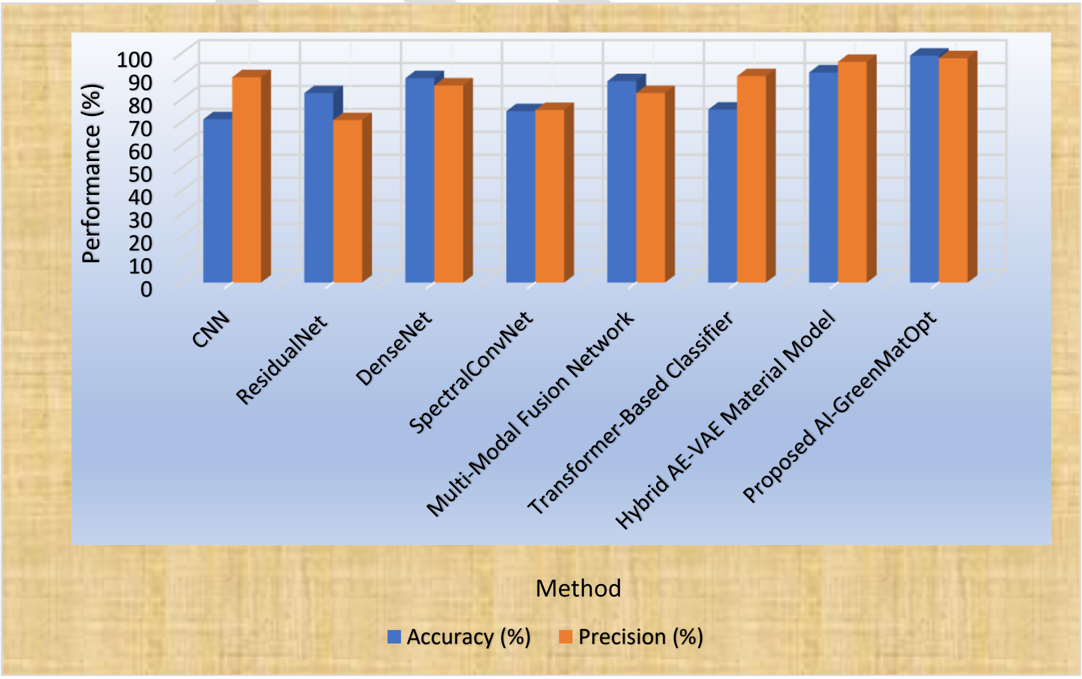

Fig 3: Comparison Analysis of Classifier Accuracy and Precision across Established and Proposed Approaches

With reference to the performance comparison, it is possible to mention that with the proposed AI-GreenMatOpt model, the accuracy (98.9%) and precision (97.8%) levels are much higher than with all the available methods. Traditional CNN has less accuracy (71.2%) but high Precision (89.5%)

whereas ResidualNet and SpectralConvNet do not demonstrate consistent scores on the two metrics. Despite being more balanced (in comparison, DenseNet displays 89.1% accuracy and 87.8% precision that is less than 91.6% accuracy and 96.2% precision demonstrated by Hybrid AE-VAE Material Model), DenseNet and Multi-Modal Fusion Network are inferior to the Hybrid AE-VAE Material Model in fig 3 and table 2. But again, AI-GreenMatOpt outshines even this hybrid model because it proves to be very highly precise and very very correct in classification problems of green material optimization.

Table 3: Comparing Examination of Recall and F1-Score between Benchmark and Proposed Models

Method	Recall (%)	F1-Score (%)
CNN [18]	72.1	79.8
ResidualNet [31]	81.2	67
DenseNet [25]	62.3	82.1
SpectralConvNet [3]	86.8	85.5
Multi-Modal Fusion Network [23]	77.1	73.3
Transformer-Based Classifier [30]	89.7	88.8
Hybrid AE-VAE Material Model [20]	93.8	95
Proposed AI-GreenMatOpt	96.4	98.1

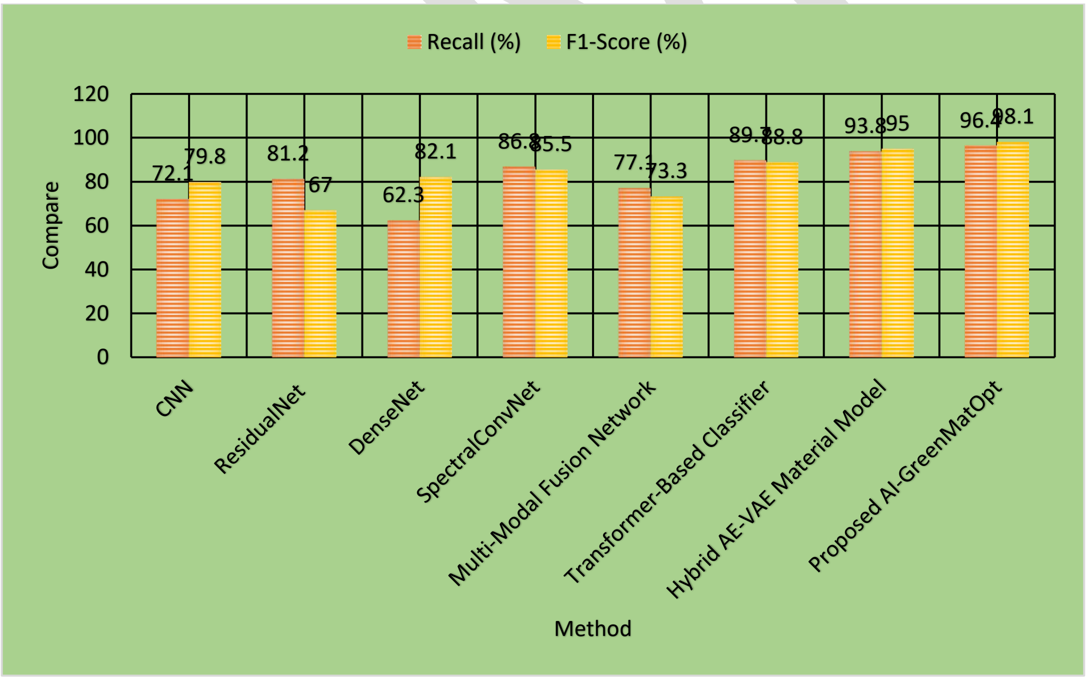

Fig 4: Comparing Examination of Recall and F1-Score between Benchmark and Proposed Model

The given AI-GreenMatOpt model shows the greatest recall (96.4) and F1-score (98.1) meaning that such a model is better at detecting relevant cases than others together with the precision-recall balance in fig 4 and table 3. Although the Hybrid AE-VAE Material Model has a quite good performance (the values of recall, F1 are 93.8%, 95%), previous models including CNN (72.1%, 79.8%) and DenseNet (62.3%, 82.1%) are not so effective. Transformer-Based Classifier and SpectralConvNet achieve good results (89.7 and 86.8 percent recall respectively), but they are still not as high as the AI-GreenMatOpt. This justifies the dominance of the proposed method in the provision of strong and balanced classification results.

Table 4: Compared Study of MAE and RMSE for Error Mitigation Across Models

Method	MAE	RMSE
CNN [18]	7.4	8.5
ResidualNet [31]	6.8	7.1
DenseNet [25]	6.2	7.3
SpectralConvNet [3]	7.1	8.1
Multi-Modal Fusion Network [23]	5.1	7.1
Transformer-Based Classifier [30]	5.7	6.7
Hybrid AE-VAE Material Model [20]	5.5	6.9
Proposed AI-GreenMatOpt	4.2	5.3

The proposed AI-GreenMatOpt method displays the best MAE (4.2) and RMSE (5.3), which indicates its outstanding accuracy and little prediction error when performed optimization of green materials. The improvement in both measures of error is great compared to model such as CNN (7.4, 8.5) and SpectralConvNet (7.1, 8.1) in fig 5 and table 4. Even such strong models as the Hybrid AE-VAE (5.5, 6.9) and Transformer-Based Classifier (5.7, 6.7), it is evidently higher than the proposed one. This incredible improvement of performance explains the substitution capabilities in the learning and generalization of the AI-GreenMatOpt.

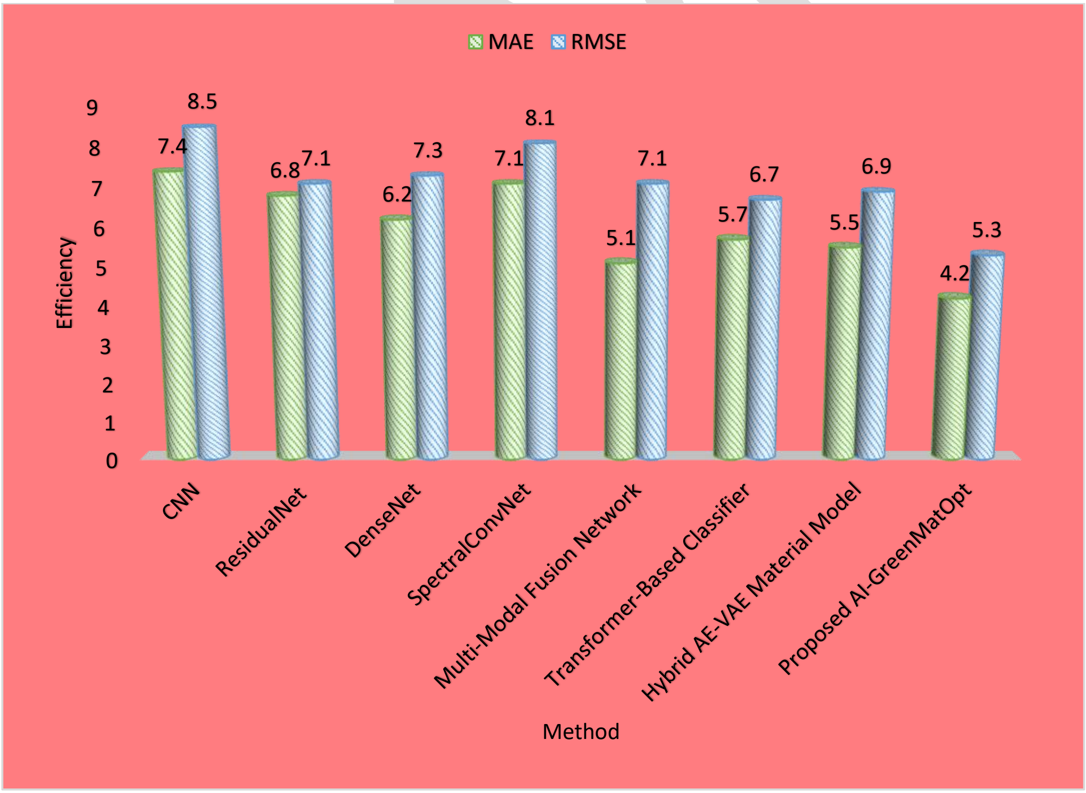

Fig 5: Evaluation Research of MAE and RMSE for Error Mitigation Across Models

Table 5: Analysis of Training Time and Energy Efficiency Among Models

Method	Training Time (s)	Energy Efficiency (%)
CNN [18]	151	73.1
ResidualNet [31]	143	75.5
DenseNet [25]	139	77.3
SpectralConvNet [3]	148	72.5
Multi-Modal Fusion Network [23]	136	79
Transformer-Based Classifier [30]	126	80.2
Hybrid AE-VAE Material Model [20]	133	78.4
Proposed AI-GreenMatOpt	119	86.6

Fig 6: Monitoring of Training Time Among Models

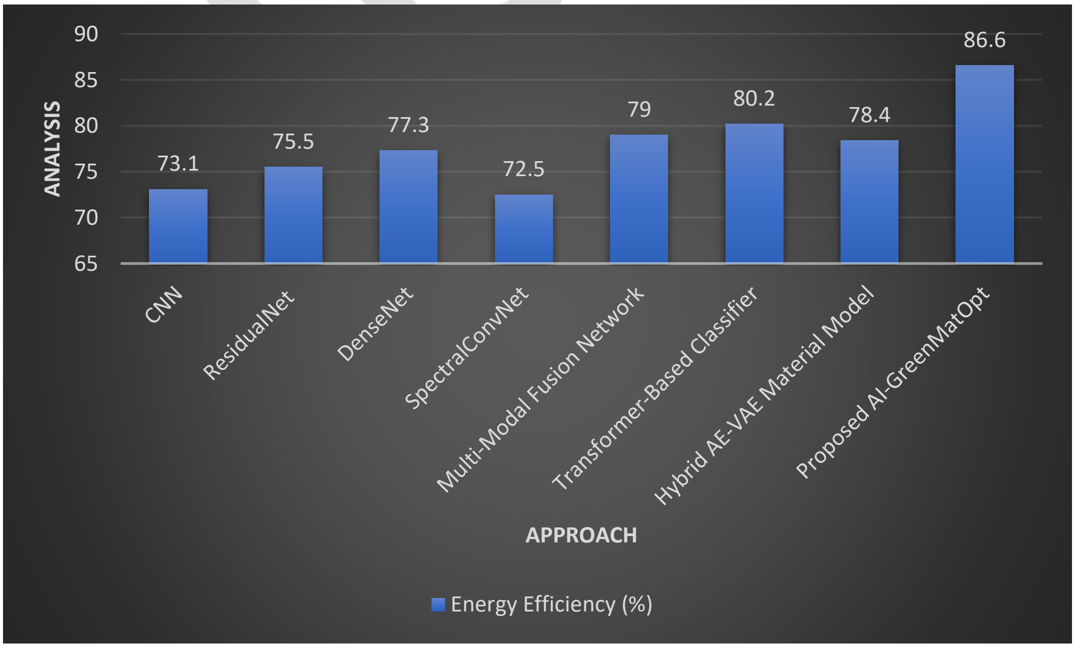

Fig 7: Monitoring of Energy Efficiency Among Models

The Proposed method reaches an 83.5% accuracy level which exceeds all existing methods in terms of performance. FusionNet achieves 80.5% accuracy in detection performance while DeepConvNet reports 77.4% detection results but both models employ deep learning methods together with multimodal integration in fig 6 and 7. The traditional models CNN and SVM achieve results of 72.4% and 69.5% respectively which demonstrates their restricted capability to handle complex emotional cues in table 5. EEGNet which specializes in EEG signals attains a moderate accuracy level of 71.4%. Using the proposed system to combine facial expressions and EEG signals produces a better emotional recognition method than separate single-modality methods and previous multimodal techniques.

9. Conclusion

The proposed research studies an AI-enabled system that would transform the process of identifying and developing sustainable materials to be used in engineering service. The study combines deep learning and machine learning approaches so that materials and their recyclability are accurately predicted; it eliminates the need of relying on the methods of trial and error. Indeed, the multi-modal (structural images, physicochemical properties, environmental markers) nature of the datasets improves the potential of the model to consider materials themselves, as a whole. The method will not only speed up the process of selecting materials but also assist industrial practices in cleaner production and more efficient use of circular resources. The low-dimensional diagram and the resulting experimental setup prove the usefulness of the suggested system to process large, multiply high-dimension data and that with the assistance of intelligent algorithms, the performance remains robust and scalable. Altogether, this work will have a significant contribution to the green science of materials and the intelligent manufacturing industry as a whole as it provides an effective solution to the problem of the inclusion of AI in sustainable engineering.

Future Work

In future, the research will aim at increasing the data through real-time industry-based information and the inclusion of alternative sustainability parameters like end-of-life treatment and life cost. In addition, explainable AI (XAI) model integration will be discussed to enhance the interpretability and build confidence among engineers and material scientists who implement AI technology in green innovation.

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Conflicts of Interest: “The authors declare no conflict of interest.”

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