

# Research Advances on the Role of Deep Learning in Materials Informatics

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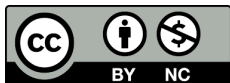
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## ABSTRACT

Deep materials informatics is a rapidly evolving field that employs deep learning techniques to develop predictive models for materials science. It involves the use of large datasets, advanced algorithms, and high-performance computing to extract key features from complex materials data. The aim of deep materials informatics is to speed up the process of locating materials with desired attributes, by taking advantage of machine learning. There are numerous applications of this technology, and it can forecast the properties of materials at all levels - from the atomic to the macroscopic. For instance, deep materials informatics are used to predict the electrical, thermal and mechanical characteristics of materials, which are critical for designing new materials for various applications. This paper offers a thorough examination of the fundamentals of deep learning, its benefits and drawbacks, and its current usage in the analysis of numerous materials datasets. Additionally, it can be utilized to optimize the processing parameters for creating materials with desired characteristics.

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## 1. INTRODUCTION

In the current age of massive data, the amount of information gathered from experiments,

simulations, and other sources has created the emergence of data-driven science. Advanced techniques for data-driven analytics are necessary to find useful information from the

data, which in turn can aid in accelerating materials discovery and realizing the Materials Genome Initiative (MGI) [1]. This fourth paradigm of science uses ML and data mining approaches to uncover actionable understandings from the data, as illustrated in Figure 1 [2].

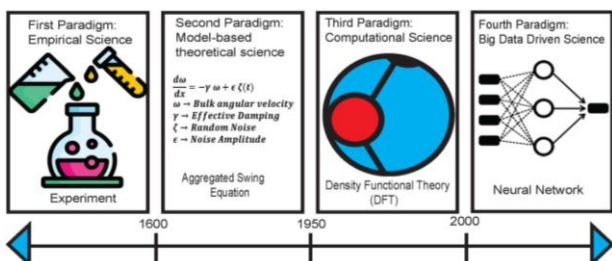


Fig. 1. The four approaches of scientific exploration as they relate to materials [2].

Researchers in materials science and engineering use experiments and simulations to try to comprehend the processing-structure-property-performance (PSPP) relationships, which are not thoroughly understood [3]. Historically, experiments were the primary method for locating and characterizing new materials. Despite its potential, this method requires a great deal of equipment and resources and can take a protracted period to yield results; thus, discoveries often occur by accident or intuition. A computational revolution in materials science was driven by the emergence of computational techniques, such as molecular dynamics, density functional theory (DFT) [4,5], and Monte Carlo simulations, which enabled researchers to investigate the phase and composition space more effectively. The PSPP relationships are integral to the study of materials and their properties. As depicted in Figure 2, the cause-effect relationships of science flow from left to right, and the goals-means relationships of engineering flow from right to left [2].

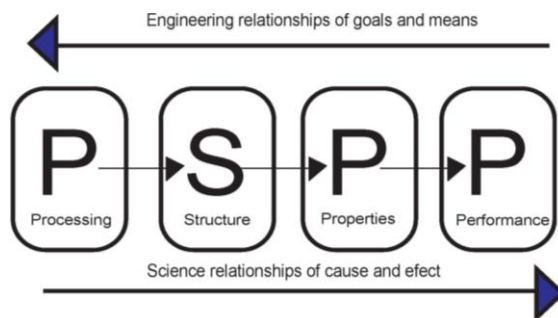


Fig. 2. The interplay between engineering and materials science. This involves science moving from the left to the right, and engineering from the right to the left [2].

Proper knowledge of complex systems must be obtained to effectively explore and develop novel materials with the preferred characteristics. Combining experiments and computer simulations have enabled us to reduce the time and cost of materials design, [6-9], and the progress in computing power and development of efficient codes have allowed for computational high-throughput studies [10] of large material groups. These large-scale simulations and calculations, together with experimental high-throughput studies, [11,12] are providing a vast amount of data that make it possible to use machine learning in materials science. The lengthy and intricate process has given us essential lessons that can be utilized in materials science to generate successful outcomes. Fourth paradigm science data-driven methods are being employed in various domains, for instance, marketing, healthcare, climate science, bioinformatics, social media, materials science, and cosmology. Recently, Deep Learning has shown itself to be a successful and popular tool in data-driven analytics, particularly when applied to Materials Informatics. This paper will provide an overview of Deep Learning, its challenges and potential, before demonstrating examples of Deep Materials Informatics. Additionally, it will discuss the exploration of PSPP linkages in materials. These include an overview of workflow [13] and learning the chemistry of materials from elemental composition [14], predicting properties based on structure, [15,16] crystal structure prediction [17], multiscale homogenization [18,19] and localization [20] of high-contrast composites, structure characterization [21,22] and quantification, [23,24] and microstructure reconstruction [25] and design [26]. We also provide a glimpse into the future of deep materials informatics and wrap up the paper with a summary and conclusion.

## 2. OVERVIEW OF DEEP LEARNING

Deep learning, a family of techniques in ML and AI, is a re-examination of neural networks (NNs) which were theorized in the 1980s [27,28]. The advent of big data and big computing has enabled these networks to become deeper, and they are capable of learning and representing a wide selection of nonlinear functions [29]. Deep learning has been a powerful tool for automating the extraction of meaningful data from large datasets and has resulted in remarkable progress in a number of areas, such as computer vision [30,31] and speech

recognition [32,33]. We will overview the deep learning's benefits and drawbacks, then discuss the constituent part of a deep NN, and at last, review some of the networks which are used for deep materials informatics.

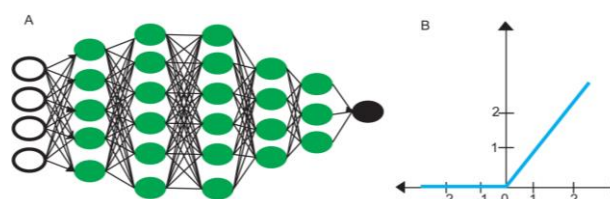
When compared to traditional ML methods, deep learning has several advantages. By using a hierarchical approach, it can identify pertinent features in data without manual feature engineering. Deep learning, with its ability to eliminate the need for feature engineering, is particularly advantageous when dealing with large datasets. Moreover, deep learning is more accurate for massive data than traditional machine learning models, which reach their limits much faster. Once the neural network is trained, it also has the advantage of being able to make predictions quickly and with great precision.

Deep learning has many advantages over traditional ML techniques, yet, in certain cases, there are still properties that complicate its usage. Below are four of the major challenges of applying deep learning:

1. Lack of sufficient training data: Data used in deep learning is typically large, curated and labelled, though this is a rarity in many scientific and engineering fields such as materials science [2].
2. Computing power: Creating deep learning models necessitates a lot of computing capabilities and can take an extended period to finish when working with large datasets, even when utilizing the most up-to-date hardware. Research is ongoing in the realm of parallelizing neural network training algorithms [34,35].
3. Network architecture search: Since neural networks are composed of interconnected neurons, there are a number of possibilities for the network architecture, and though there are some general guidelines for choosing an architecture for a given problem, there is no formal method to determine the optimal architecture for a task; this is an open research topic [36].
4. Model interpretability: Deep learning-based models are usually seen as black-box models due to their complexity, and though there

have been some attempts to better understand the workings of the neural network, they are not as easily interpretable as some traditional statistical models such as linear regression [37].

Neurons, which are the basic components of Artificial Neural Networks (ANNs), take their design from biological neurons found in the human brain. Each neuron processes multiple inputs and produces an output based on a weighted sum of the inputs, and the output is then transformed by a non-linear activation function (AF). ANNs commonly employ rectified linear units (ReLU), linear, sigmoid, and leaky ReLU activation functions. A fully-connected artificial neural network (ANN) uses the ReLU activation function, as demonstrated in Figure 3.



**Fig. 3.** (A). Depiction of a deep ANN (fully connected) with one output, four inputs, and five layers found between the input and output layers with an inconsistent amount of neurons. (B). The graph utilizes the ReLU activation function [24].

Deep learning networks are a kind of ANN that consist of two or more hidden layers; a hidden layer is situated between the input and output layers. The structure of the network is established by how the neurons are interconnected. In addition, weights are assigned to the edges between neurons and are adjusted during the training process of the ANN so that the outputs become more accurate. To use an artificial neural network (ANN) to make predictions, the input data is passed through the network to yield the outputs. The loss or errors are then calculated, and the weights of the connections between neurons are adjusted in order to minimize the error, a process known as back-propagation. One pass of the entire training data is referred to as an epoch (which consists of one or more batches and a part of the dataset is used to train the neural network) and it is repeated iteratively until the weights have converged [38]. Normalization of the inputs and at times the inputs of the internal layers are carried out (known as batch normalization) to stabilize the artificial neural networks. Dropouts are a noteworthy and valuable idea in Artificial Neural Networks (ANNs) that involve randomly

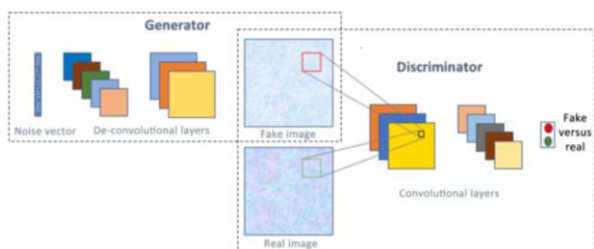
turning off certain neurons when undergoing a backward or forward pass. This is a regularization method for reducing overfitting, and it is also found to be an effective method for approximating multi-model averaging [38].

## 2.1 Convolutional Neural Network (CNNs)

A Convolutional Neural Network (CNN) is an Artificial Intelligence algorithm that is capable of analyzing an input image, determining the relative importance (via learnable weights and biases) of various objects and features, and differentiating among them. It is composed of three main hidden layers: a convolutional layer, a fully connected layer, and a pooling layer. The convolutional layer uses numerous kernels on the image to generate abstract features, which then serve as inputs for the next layer. The outputs of this layer are then condensed into a one-dimensional vector, which is used as the input for the fully connected layers, producing the final prediction. The most common type of CNNs are 2-D CNNs which work with 2-D input matrices, however, there are other variants such as 1-D and 3-D CNNs which take 1-D vectors and 3-D matrices respectively as input, and graph CNNs [39,40] that can work with graphs as input.

## 2.2 Generative Adversarial Networks (GANs)

A generative adversarial network (GAN)[41] is a sophisticated deep learning architecture that has been developed recently, based on game theory. Figure 4 illustrates two neural networks paired together in a competitive way.



**Fig. 4.** A GAN is composed of two neural networks, a generator and a discriminator, and when given the right instruction, it has the ability to create lifelike images/data from random noise [24].

The first one, labelled as the generator, takes a random noise vector and increases its resolution to produce a synthetic image. The second is a convolutional network, referred to

as the discriminator, which takes a picture as input and reduces its resolution, generating a probability distribution to determine if the image is genuine or false. It can be likened to a criminal creating counterfeit money, with the discriminator as the police tasked with recognizing the false currency. As the two neural networks are trained, they become more and more proficient, till they reach the Nash equilibrium [42]. GANs have been utilized in a variety of image analysis applications, such as high-resolution image synthesis [43], text-to-image synthesis [44], image editing [45], blending [46], inpainting [47], and beyond image domains, like music generation [48].

## 3. THE APPLICATION OF DEEP LEARNING TO UNDERSTAND PSPP RELATIONSHIPS IN MATERIALS SCIENCE

By examining how deep materials informatics has been used to explore PSPP links through inverse and forward models, we can gain insight into the specific characteristics of deep learning in the materials sector.

### 3.1 Understanding Material Chemistry Through Elemental Analysis

Jha et al. recently developed a neural network called ElemNet which requires only the elemental composition of a crystalline compound as input and predicts its formation enthalpy [14]. This deep learning method does not require any feature engineering, which is a major benefit when compared to traditional machine learning algorithms. To test the efficacy (considering its mean absolute error (MAE)) of ElemNet, a dataset from the Open Quantum Materials Database (OQMD) of approximately 276,000 compounds were used. The Random Forest model - well-known for being the most efficient of the traditional machine learning approaches - achieved a 0.157 (electron volts per atom) MAE when only using elemental components as features. By including composition-derived physical attributes, however, the MAE was reduced significantly to 0.071 electron volts per atom. On the other hand, ElemNet attained an even lower MAE of 0.055 electron volts per atom when only the elemental compositions were considered. Thus, this result indicated that the ElemNet was more successful than the

traditional machine learning algorithms, even when physical attributes were present. In addition, ElemNet was successful in predicting convex hull phase diagrams for unseen material systems when two specifically designed training-test splits were evaluated. Further research into the effects of varying training set sizes demonstrated that ElemNet was more successful than RF when over 4000 compounds were present. With a training and test set of 250,000 compounds each, ElemNet took approximately 7 hours to train on a GPU but was much quicker when it came to prediction time, requiring 0.08 and 9.28 seconds on a GPU and CPU respectively.

Jha et al. [14] investigated the workings of ElemNet to explain its successful results. It was examined that the representations of the network had learned and studied the activations of the network when given certain inputs. It was revealed that ElemNet had taught itself features that are related to chemistry (such as element similarity and interactions), despite not receiving any periodic table information during training. When using Principal Component Analysis (PCA) to map the activations of the second and first layers generated by Alkali Metals (Caesium, Lithium, Sodium, Potassium, and Rubidium) into a two-dimensional space, the results were arranged in a straight line. Experiments with binary mixtures of Alkali Metals/Alkaline Earth Metals and Chalcogens/Halogens elements conducted through the model showed that the charge-unbalanced and balanced compositions clustered independently in the eighth layer of ElemNet. ElemNet employs a deep learning approach which is akin to that used for image recognition. In this process, initial layers are designed to recognize fundamental features such as corners and edges, after which, for instance, 'shape', a more complex element can be identified in subsequent layers. This technique proved to be especially accurate and rapid, allowing the authors to explore the quaternary space, analyzing nearly 500 million compounds. Their findings included a variety of hitherto unseen systems with at least one potentially stable compound. To reinforce the reliability of the results, some of these compounds were found to be present in the Inorganic Crystal Structure Database (ICSD) but were missing from the OQMD.

### 3.2 Crystal Structure Examinations for Predicting Characteristics of a Material

Even though composition-based models are highly accurate, the structure is still a major factor in materials because different polymorphs and allotropes can have different characteristics with the same chemical makeup. Therefore, it is necessary to create models that are sensitive to structures for predicting material properties. Several research projects have been conducted, using diverse sets of features to represent structure information [49-52] for the ML algorithms to build predictive models. Recently, deep learning has been used directly on the crystal structure, as discussed by Xie and Grossman [15]. A CNN framework was devised to extract material properties from the connections between atoms in the crystal. To begin, the crystal composition is expressed as a crystal graph, in which the atoms in the unit cell are represented as nodes. A CNN is then implemented on the graph, consisting of pooling layers, fully connected layers, and convolutional layers, in order to draw out the best representations for modelling the specified characteristics. The database contained 46,744 materials from the Materials Project [53] which spanned 87 elements, 7 lattice systems, and 216 space groups. A model was initially used to predict formation energy with a mean MAE of 0.108 electron volts per atom. This model had two layers, and the same weights were used for all neighbouring atoms in each layer. This was improved by the introduction of a convolution function that considered the varying interaction strength between neighbouring atoms, resulting in an MAE of 0.039 electron volts per atom. Additionally, a similar framework was then used in determining other density functional theory-computed properties like shear moduli, absolute energy, bulk moduli, Fermi energy, Poisson ratio, and band gap from the Materials Project. Recently, Ye et al. [16] demonstrated that through the use of artificial neural networks and only two descriptors, the density functional theory formation energies of C3A2D3O12 garnets and ABO3 perovskites can be accurately predicted, with mean absolute errors of 0.007-0.010 electron volt per atom and 0.020-0.034 electron volt per atom, respectively. The two descriptors are (1).

Pauling electronegativity. (2). Ionic radii of the elements involved. Ye et al found a way to model total cation disorder for mixed garnets its type of species in D, A, and C sites are more than one, using an averaging technique and a binary encoding scheme that only slightly reduced accuracy.

### 3.3 Prediction of Crystal Structure

Foretelling crystalline formations is a difficult task in the realm of materials science, akin to the way protein structure prediction is carried out in bioinformatics. Breaking the problem down into two parts, the first step is to generate possible structures and the second part is to evaluate them to determine which is the most probable. Usually, evolutionary algorithms using random starting points are used for the structure generation step and quantum mechanical methods assess the structures. Recently, Ryan et al. applied deep learning to crystal structure prediction, particularly for structure evaluation [17]. The problem in predicting crystal structure was modified by Ryan et al. by predicting the likelihood of each atomic site. This was done by multiplying the chance of the atom appearing in a certain spot. To do this, data from the Crystallographic Open Database and ICSD, which consists of around 704,000 distinct sites in around 52,000 crystal structures, was used. In order to capture the local environment surrounding each site, the model was trained using an input representation of atomic sites that was composed of normalized atomic fingerprints. The input featured properties like three-dimensional data retention, translational invariance, and a fixed number of dimensions which enabled the model to master structural layouts as opposed to specific crystal formations. The deep neural network was made up of three separate networks. To start with, a forty-two-layer convolutional variational autoencoder compressed the 3072-dimensional atomic fingerprints into sixty-four-dimensional latent representations. Afterwards, a 5-layer sigmoid classifier was used to predict the element combinations likely to form certain structural topologies based on latent representations. This was then fed into a five-layer auxiliary softmax classifier with batch normalization and 118 output neurons, thus changing the element prediction query into a

118-class classification difficulty. When the test set was compared to its baseline value (which was 20 per cent of the full atomic fingerprint data), the average level of inaccuracy was 31 per cent, an impressive result for such a complex system. Blunders that were chemically logical made by the model were discovered to be chemically (for instance 4f and 3d elements). Also, the t-distributed stochastic neighbour embedding (t-SNE), which is mostly used for exploring data and representing high-dimensional data, was applied to the sigmoid classifier weights of the elements shown. This resulted in groupings similar to those of the periodic table. This indicates that the deep learning model was capable of understanding periodic trends and chemical similarities without any explicit instruction, just like the ElemNet model [14] did with composition data. Turning to the crystal structure prediction problem, Ryan et al [17] used a list of known structure types as the basis for creating new crystal structures, and the deep learning model to evaluate the structures. The generator used 51,723 known structures as a base and combined substitution across all elements to generate a total of 2,703,834 ternary and 623,380 binary possible crystal structures. This is a unique process that has never been done before. Ryan et al [14] combined a structure generation technique with deep learning based structure evaluation to make crystal structure predictions. A holdout test set of 5845 crystal structures was employed to evaluate the performance of the model. It was found that the correct structure was the highest-ranked choice 27% of the time, and it was part of the top 10 predicted structures 59% of the time. The authors of this study demonstrated the capacity of deep learning models to autonomously gain the knowledge associated with chemistry from geometric and topological data, as well as how it can be applied to the intricate undertaking of crystal structure prediction. They demonstrated this in a case study of Manganese–Germanium and Lithium–Manganese–Germanium systems, which revealed unique, novel chemical compositions with matching predicted structure templates. Despite the fact that the accuracy of the predictions may be underestimated due to the isostructural crystal structures, this study demonstrates the potential of deep learning models to facilitate crystal structure prediction.

### 3.4 Relationship Between Localization and Homogenization at Multiple Scales in High-Contrast Composites

Examining the connection between structure and properties at various lengths scales, an exploration of deep learning to three-dimensional microstructure data of two-phase composites is conducted in this section. Homogenization is the process by which microstructure information is transferred from smaller scales to larger ones, such as predicting macroscale properties based on microstructure information. Localization is when salient microstructure information is transferred from larger scales to smaller scales, like how a load is distributed in a material's microstructure under macroscopic loading conditions. These homogenization and localization connections are modelled using numerical techniques [24]. In recent years, Materials Knowledge Systems (MKS) [54] have been created to understand localization connections, which are non-iterative series solutions using calibrated Green's function-based kernels, as well as ML-based methods which require feature engineering to capture the local microstructure neighbourhood.

Yang et al. [18] proposed a feature-engineering-free deep learning-based homogenization solution to predict macroscale effective stiffness in two-phase composites with a contrast of 50. By employing 3-D convolutional neural networks (CNNs) to map microstructure information to effective stiffness, a homogenization link was established utilizing a dataset of 8550 simulated  $51 \times 51 \times 51$  3-D microstructures (known as MVEs). The most efficient deep learning network was identified as a 14-layer model containing five convolution blocks (each consisting of a convolution layer followed by a pooling layer) and two fully connected layers, with 3.8 million trainable parameters. This network was used to compute the effective stiffness through micromechanical finite element simulations with periodic boundary conditions. The accuracy of the deep learning model (MAE of 1.04 GPa or 3.10%) was significantly better than simple physics-based approaches or rule of mixtures method (MAE of 15.68 GPa or 46.66%) and sophisticated physics-inspired data science approaches that utilize principal component analysis (PCA) on two-point statistics as input features for regression [55] (MAE of 2.28 GPa or

6.79%). Moreover, another recent work [19] on using deep learning for homogenization has shown that the filters/kernels learned by the CNN during training can be interpreted as microstructure features that the model learns to be influential for improving the macroscale property of interest. The inverse problem of design exploration could be significantly aided by this approach, ultimately providing feedback to inform materials design.

Yang et al. [20] proposed a deep-learning technique that does not require any feature engineering for localization. They experimented with two datasets composed of 2500 MVEs (contrast-10) and 3000 MVEs (contrast-50) of size  $21 \times 21 \times 21$ , with periodic boundary conditions and varying volume fractions. To represent each voxel, a 3-D neighbourhood of size  $11 \times 11 \times 11$  was used, which would have been computationally expensive if 3-D CNNs were used. The authors employed a 2-D CNNs approach instead of 3-D CNNs. This entailed treating the 3-D image of  $11 \times 11 \times 11$  as 11 channels of a 2-D image of  $11 \times 11$  which was perpendicular to the maximum principal strain direction. The CNN architecture featured six layers, with two fully-connected layers and two convolution layers. The accuracy of the deep learning model was compared to the MKS method [47], as well as single-agent [56] and multi-agent [57] ML-based methods. The single-agent and multi-agent methods recorded a mean absolute strain error (MASE) of 13.02% and 8.04%, respectively, on the contrast-10 dataset. The MKS method, however, yielded a MASE of 10.86%. The deep learning CNN model, though, had a clearly better MASE of 3.07%. The MKS method had a MASE of 26.46% on contrast-50, which was much higher than the 5.71% MASE obtained by the deep learning model. An analysis of what CNN learned showed that the impact of different level neighbours decreases with increasing levels of neighbours, which is in accordance with existing domain knowledge.

### 3.5 Quantification and Characterization of Microstructure

Materials characterization is a process that can help us understand the structure of a specific material [58], By using advanced techniques at varying lengths and times, such as different microscopies and spectroscopies, materials

imaging has become more prolific. Electron backscatter diffraction (EBSD) is one of these techniques that can be used to measure the three Euler angles of a crystalline material which are represented by  $(\varphi_1, \Phi, \varphi_2)$  [59]. Known as EBSD indexing, the problem of learning orientation angles from an EBSD pattern is an inverse structure characterization. The Hough transform-based method, which is often used commercially, is effective but can be impaired by noise in the pattern. An alternative method of indexing is dictionary-based, which is a strong and effective method of finding the nearest neighbour. The results of this search are the angles of the EBSD pattern closest to the query. Unfortunately, this method is computationally expensive.

Liu et al. recently tested a deep learning method to index EBSD patterns, training a CNN model on 300,000 of the 333,227 that are simulated with EBSD patterns (60 x 60 grayscale images). Despite this, the performance of the CNN model could have been improved had it been trained using the entire lexicon and optimized for the discrepancy between the predicted and actual orientations. Jha et al. [22] addressed these limitations in their research by training their CNN model on two dictionaries comprised of 374,852 EBSD patterns (including 1000 independent simulated EBSD patterns) and optimizing for the mean disorientation error by creating a differentiable approximation to the disorientation function. This network, comprised of 17 layers and roughly 200 million parameters, was able to beat the dictionary approach by 16%. The mean disorientation was  $0.548^\circ$  for the network, while the dictionary technique yielded  $0.652^\circ$ .

DeCost et al. [23] presented a deep learning solution for the quantitative analysis of ultrahigh carbon steel microstructure, consisting of two tasks: (i) segmentation of steel micrographs into four regions (grain boundary carbide, spheroidized particle matrix, particle-free grain boundary denuded zone, and Widmanstätten cementite); and (ii) segmentation of cementite particles within the spheroidized particle matrix. This was accomplished by using the PixelNet [60] architecture, which represents each pixel by the concatenation of its representations in each convolutional layer, and then applying a Multilayer perceptron (MLP) to map the

hypercolumn pixel features to the corresponding target. The convolutional layers were based on the pre-trained VGG16 network [61], and the MLP layers were trained from scratch, with batch normalization, dropout, weight decay regularization, and data augmentation. The segmentation model performance was tested with focal loss (FL) and cross-entropy (CE) classification loss on a dataset of 24 micrographs. While the model was successful in accurately categorizing spheroidite and particle segmentation, it encountered difficulties when trying to recognize particles of less than 5 pixels in radius. This indicates that higher-quality input is essential for training the model. Patton et al. [36] recently developed MENNDL, a 167-petaflop deep learning system for automated raw electron microscopy image-based atomic defect identification and analysis on a supercomputer. An asynchronous, parallel, scalable, genetic algorithm combined with a support vector machine enables the system to swiftly identify the optimal network and can generate and evaluate several deep neural networks (DNNs) comprising various hyperparameters and architectures in a few hours. This deep learning network further facilitates the development of a mapping of atomic transformation pathways, a library of imperfections, examination of local atomic environment distortions near defects, and automated selection of the most favourable area in the sample for measurements or manipulations without human intervention, forming the base for an independent microscope.

### 3.6 Design and Reconstruction Microstructure

Reconstructing a disordered heterogeneous material's structure with limited structural information about the original system is still a significant issue in modelling heterogeneous materials [61]. A deep transfer learning method was developed by Li et al [25] to generate statistically similar microstructures of any material system from only one provided microstructure. In their technique, the input microstructure with k-labelled materials is initially encoded into a three-channel (RGB) form to be used as an input to a pruned version of a pre-trained CNN known as VGG19 [62]. Also sent to the pruned VGG19 network is a randomly initialized RGB image, which will be iteratively changed as it is reconstructed into the encoded microstructure. The loss function to be

minimized is the difference of Gram-matrix (a measure of the texture of a given image) [63] between the activations of the original and reconstructed microstructure, summed up over chosen convolutional layers of the pruned VGG19. The weights of the network are fixed, thus requiring the optimization of the pixel values of the microstructure reconstruction. Gradients of the loss function are calculated through backpropagation and then used in a nonlinear optimization algorithm to iteratively update the pixel values until convergence is attained. To achieve the desired result, the authors carried out a post-processing step with simulated annealing after decoding the reconstruction through k-means clustering. This clustering divides the pixels into k groups, the number of which corresponds to the number of material phases in the original microstructure. However, it does not guarantee that the volume fractions will match the original microstructure. To remedy this, simulated annealing was employed to switch the phase label of some boundary pixels in order to make the volume fractions of the original and reconstructed microstructures equivalent.

Yang and Li et al. [25,26] recently developed a deep adversarial learning methodology of GANs for a low-dimensional and non-linear embedding of microstructures for microstructural materials design. This approach was tested on various structural morphologies, such as carbonate, polymer composites, sandstone, ceramics, a block copolymer, a metallic alloy, and three-phase rubber composites, and was found to be more efficient than other methods (decision tree-based synthesis [64], Gaussian random field [65], two-point correlation [66], and physical descriptor [67] in four out of the five material systems. After training a GAN on 5000 synthetic microstructure images generated with the GRF method, it was then used to randomly sample a latent variable vector and generate new images. The realism of the images was verified by their lineal-path correlation and two-point correlation functions. To prove the power of the design optimization framework, a GAN was utilized together with Bayesian optimization and rigorous coupled wave analysis so as to simulate the optical absorption performance of the microstructure in question. The authors observed that the GAN-generated microstructures had an optical performance that was 4.8 per cent superior to randomly sampled

microstructures and 17.2 per cent superior when optimized using Bayesian optimization. The generator, which was trained, was capable of creating microstructures of any size and the discriminator could be employed to initially train models for predicting structure-property relationships.

#### **4. PROSPECT AND FUTURE IMPACT**

Deep learning is a rapidly expanding field of research which has been garnering considerable attention, leading to cutting-edge algorithms being created at an astonishing rate. Below is a summary of the essential principles of deep learning as they relate to material informatics, which is likely to have a large influence on how data-driven approaches are used in materials science.

##### **4.1 Other Forms of DNNs**

This paper has discussed three different types of deep-learning neural networks: CNNs, GANs, and MLPs. However, there are also many other kinds of networks that can process different forms of data. For instance, recurrent neural networks are designed for sequence data (or temporal data) of different lengths, and are commonly used for speech recognition [68], natural language processing [69], and recently in materials informatics [70,71]. Geometric deep learning has recently been developed as a form of deep learning capable of dealing with non-Euclidean data, for example, nodes and edges in graphs, which cannot be handled by standard deep learning kernels, such as convolution. This method is applicable in quantum chemistry [72,73], particularly in analyzing data from molecular dynamics simulations.

##### **4.2 Transfer Learning**

Deep learning traditionally needs a great amount of data, yet transfer learning enables its use even in situations with a limited amount of data. This is done by taking the knowledge obtained from a deep learning model that was built with a much larger dataset related to a different problem and creating a new model with a much smaller dataset for the current problem. This approach is anticipated to be especially helpful for materials informatics, as the datasets used are usually much smaller than those used in other areas such as cosmology, bioinformatics, and social media.

Transfer learning is also widely used for image classification, where pre-trained deep learning models, such as VGG [62] trained on the large ImageNet [74] database (containing more than 14 million labelled images), can be used to extract important features from small datasets and build ML models [75].

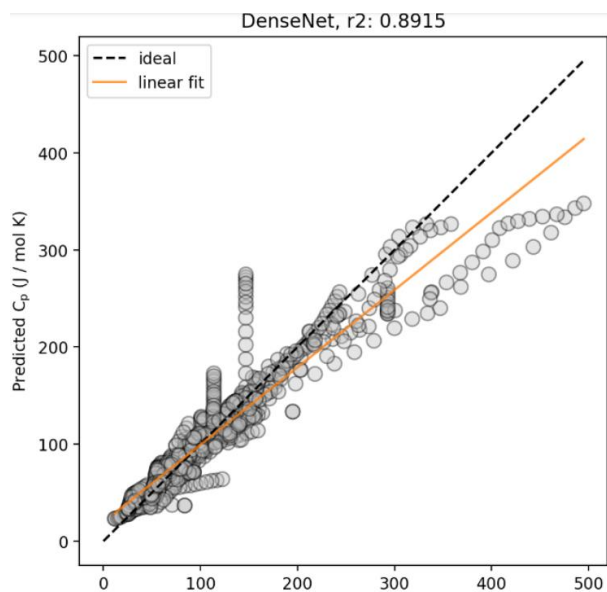
#### 4.3 Active Learning and Uncertainty Quantification

In the future, Uncertainty Quantification (UQ) will become increasingly significant in the realm of materials informatics predictive analytics. UQ enables the precise determination of uncertainty for ML model predictions, within a specified confidence range. An ensemble data mining approach [76] is one common methodology for UQ in materials informatics, where multiple predictive models are constructed for the same task by using different techniques on the same data or the same technique on different subsets of data, with the final prediction being calculated with the individual predictions, such as by their mean. One can assess the degree of instability by computing the standard deviation of individual forecasts, or by combining it with the error of the model's prediction. An alternate method is through deep learning models, which use dropout during the training of neural networks to make the model more generalizable and to simulate model ensembling [38]. At the assessment phase of the model, certain neurons are randomly deactivated via dropout, which can cause the same input to produce various results each time it is processed. This set of predictions can then be used to generate uncertainty estimates, similar to ensemble learning models or more sophisticated methods [77]. At UQ, there is a strong emphasis on active and reinforcement learning. In these methods, an algorithm is employed to determine which unlabeled inputs should be labelled to increase the precision of the model or to decide the ideal action in a given context to acquire the highest reward. Data-driven material discovery has practical implications. By using a set of experimental or simulated data, it is possible to predict which experiment or simulation should be carried out next to upgrade the predictive model. By using this updated system which incorporates active learning, the search for the ideal product with the necessary qualities can be hastened. This diminishes the number of experiments needed to reach a conclusion.

#### 4.4 Interpretability of Model

The importance of being able to interpret models has been a major concern when it comes to applications like finance, self-driving, and materials engineering, where a single incorrect positive result can cost dearly. Lipton [78] proposed a comprehensive taxonomy of interpretability criteria and methods, distinguishing between interpretations that are transparent to humans and those that are post-hoc explanations. Transparency refers to the comprehension of the model's training, inputs, parameters, and overall functioning, although it is typically at odds with complexity. Although some models are not easily understandable, deep trees and linear models with elaborate inputs and ensembles can be less transparent than a basic neural network that has been through minimal processing. In contrast, post-hoc analyses require comprehension of what the model has determined, making deep-learning models an ideal tool due to their extensive representations. Visualization techniques, such as t-SNE [79] or saliency maps [80], can be used to map the latent representations of a model in 2D or to identify the most influential sections of the input. Additionally, a model's low-dimensional latent representation can be used to identify the k-nearest neighbors in the training set and explain the model's decisions by showing similar examples from the training set. [78] There are several other methods and guidelines to understand deep learning networks [81]. A workflow practice of using a Python programming language in modeling using neural network / deep learning-based models is provided by Wang et al. [13] which contains training, validation, and test sets, as it is customary for a machine learning project, the dataset contains 309 columns each of which is in double data type representing an attribute of the material sample. Some data transformations were done, these included scaling and transformation. Then they proceeded to build the deep learning project, which adopted a dense fully connected neural network, The input layer of DenseNet accepts input data in the dimension of each row of the input data, which is equal to the number of features in the composition-based feature vectors (CBFV) featurization scheme. When the Oliynyk featurizer was used, the input dimension was 177. The model's input layer is the dimension of the dataset which is 309, with a hidden layer of 64 by

32 and an output dimension of 1. A dataloader class specific was defined for loading CBFV-type datasets and a batch size of 128. For the loss function and optimizers, they adopted Loss and Adam optimizer and the training lasted 500 epochs. After training the model was evaluated and got an R2 score of 0.9863, MAE of 3.7027, RMSE of 7.0814 and for the validation set, R2 score of 0.9102, MAE of 13.6182, RMSE of 23.9155 were realized, as shown in figure 5.



**Fig. 5.** Evaluation of model that predicts the heat capacity of inorganic materials [13].

#### 4.5 The Possible Effects Over Time

Material advancement is essential for the growth of the industry, and its advancement is vital for the prosperity of our society. Deep materials informatics techniques have the potential to revolutionize the field of materials science, as well as various industries. By providing the means to explore near-endless possibilities in materials, researchers can more easily identify the best options and then test them through experiments and simulations, ultimately accelerating the process of acquiring and using advanced materials while also reducing the cost of materials production. The Materials Genome Initiative (MGI) strives to identify and create innovative materials in an economical manner. Utilizing deep materials informatics could accelerate this process, thereby providing substantial advantages to businesses in numerous industries, for instance, automobiles, healthcare, transportation, construction, clean energy, and aerospace.

#### 4.6 Conclusion and Summary

Deep Materials Informatics, similar to bioinformatics of two decades ago, is still in its infancy, specifically in the area of deep learning for materials science. This paper examines the most recent developments in deep materials informatics, such as categorizing elemental composition, crystal structure, and two-dimensional and three-dimensional microstructure images. Additionally, the fundamentals of deep learning, its benefits and obstacles, the deep learning networks' various types, and the future of deep materials informatics are evaluated. With the ongoing expansion of big data and materials databases, coupled with headways in data science and deep learning techniques, there is immense potential to revolutionize the prediction of materials properties, discovery, design, and application of advanced materials. Model evaluation as done by Wang et al, was done on the test set and test R2 of 0.8919, test MAE of 14.4120, and test of 25.6550. It was realized that machine learning is better for material science because Deep learning models can rapidly analyze vast amounts of data, accelerating the discovery process. In contrast, traditional lab work often involves time-consuming experiments and manual data analysis as well as uncovering hidden patterns and relationships in data that may not be apparent through conventional analysis methods. This can lead to new insights and discoveries in material science. Deep learning models can also predict material properties and behaviors based on data, allowing researchers to explore a wide range of possibilities without extensive experimentation.

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