ARTIFICIAL INTELLIGENCE IN MATERIAL ENGINEERING

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ABSTRACT

Abstract: The role of artificial intelligence (AI) in material science and engineering (MSE) is becoming increasingly important as AI technology advances. The development of high-performance computing has made it possible to test deep learning (DL) models with significant parameters, providing an opportunity to overcome the limitation of traditional computational methods, such as density functional theory (DFT), in property prediction. Machine Learning (ML) based methods are faster and more accurate than DFT based methods. Furthermore, the generative adversarial networks (GANs) have facilitated the generation of chemical compositions of inorganic materials without using crystal structure information. These developments have significantly impacted the material engineering (ME) and research. Some of the latest developments in AI in ME herein are reviewed. First, the development of AI in the critical areas of ME, such as in material processing, the study of structure and material property, and measuring the performance of materials in various aspects, is discussed. Then, the significant methods of AI and their uses in MSE, such as graph neural network, generative models, transfer of learning etc are discussed. The use of AI to analyze the results from existing analytical instruments is also discussed. Finally, AI’s advantages, disadvantages, and future in ME are discussed.

1 Introduction:

Material Science and Engineering (MSE) is mainly concerned with four characteristics of a material. These are processing, structure, property, and performance. The key to material engineering lies in the interrelation of these four characteristics. In short, the combinations of processing, structure, property, and performance are key in material engineering. Here the structure represents the atomic arrangements of the material. Performance defines how well the material plays its role in a particular task. Properties like hardness/softness, the density of the particles, fracture toughness, resistivity, and thermal expansion are determined by the structure. These properties can be engineered by adopting appropriate processing methods. Here, the processing is a series of steps that are involved to convert a material to some useful form by tweaking the properties of the material. Engineered materials such as metals, polymers, liquid crystals, and composites are widely used in the fields such as medicine, energy, manufacturing, biotechnology, etc. Therefore, MSE is an emerging area applicable in a variety of materials for multiple disciples like medical science, biotechnology, nanotechnology, drug discovery, energy storage materials, etc.

Some of the traditional techniques used in MSE are i) Density Functional Theory (DFT) which is a simulation method that uses the quantum mechanical laws to find out the electrical properties of atoms, molecules, and solids. ii) Density Functional Perturbation Theory (DFPT) where the quantum system is studied in small perturbation mostly
used in calculating vibrational energies of phonon that can further be used to find out the physical properties. Classical force-field inspired descriptors (CFID) that represent the chemistry-structure-charge data of a material. But these traditional methods take a considerable amount of time in processing and analysis. Also, these can not be applied in all types of structures.

With years of study and experimentation on the conventional methods of property prediction, such as the empirical trial-error method, and density functional theory (DFT), researchers have collected huge data in the field of MSE. These Big data may help in designing a data-driven approach for MSE. In this regard, Artificial Intelligence (AI) can play a major role. AI is an area of computer science that leads a system to learn from data and improves performance in every subsequent iteration. The learning process starts with the observation of data to find out the meaningful features to attain the set objectives. In the last few years, with the increasing experimental and simulation-based dataset, AI and machine learning (ML) have been widely used to gain a deeper insight into the material.

1.1 A Brief discussion on existing literature on AI in material engineering:

A handful of reviews have already been made in the context of applications of AI in material engineering. For example, Kamal Choudhary et al. have discussed the available ML techniques and their libraries [5]. Chi Chen et al. have discussed the ML methods that are specifically used for energy materials [6]. Jonathan Schmid et al. have discussed the ML algorithms for crystal structure prediction [7] and Valentin Stanev et al. have discussed the AI models that are used in quantum materials [8]. Daniel P Tabor and co-authors provided a fruitful discussion on discoveries in the clean energy sector along with the state-of-the-art procedures for organic, inorganic, and nanomaterials [9]. Table 4 of the supplementary document contains the details of models that are built particularly in the field of organic, inorganic, energy storage, drug and pharmaceutical, and biomaterials. In the same work, high throughput virtual screening, genetic algorithms in the synthesis of catalysts, and ML algorithms in perovskite synthesis for photovoltaic are discussed. The challenges that are still found in the automatic synthesis of inorganic and organic molecules, the autonomous laboratories fueled by AI models for chemical synthesis, the techniques used for automatic and rapid characterization of materials, the use of autonomous robots in the laboratories for speeding up the experimentation are also mentioned with state-of-the-art works. The use of generative and discriminative neural networks in photonic devices, the types of datasets particularly used for electromagnetics, and some of the dimensionality reduction techniques are elaborately discussed by Jiaqi Jiang et al. [10]. Mohit Pandey et al. have discussed the use of Graphics Processing Units (GPU), Deep Generative Networks, and transfer learning models have shown significant acceleration in the field of drug discovery [11]. The GPU-based systems can reduce the computational cost to a great extent in comparison to the CPU in the simulation of molecular dynamics. GPU-specific quantum chemistry codes such as TeraChem are developed for simulating the entire protein structure using DFT.

1.2 AI in structural, elemental, electronic and thermal, di-electric and mechanical property prediction:

Extending the existing review of AI in MSE, we focused on AI and ML methods that are developed for various material types like organic, inorganic, energy-storage, bio, and pharmaceutical materials to predict Stoichiometric, electronic, elemental, ionic, optical, structural, and thermal properties. Recently, the Scanning Tunneling Microscope (STM) images have been used in convolutional neural networks (JARVIS-STMNet) to classify the structure of Bravais-lattices. This classification is used for phase identification, information extraction from poor resolution, etc. [12]. ML models designed using Gradient Boosted Trees (GBT) algorithm has found to be superior as compared to many other classification models in predicting the topological structure of materials [13]. The famous Random Forest algorithm is used to find out the critical temperature (Tc) value of superconductivity [14]. Again graph neural network named Atomic Line Graph Neural Network (ALIGNN) is used by Kamal Choudhary and his team to predict the structural and electronic properties and also for the quantities like adsorption isotherm of CO2 for various pressure [15]. A schematic of the ALIGNN is shown in Fig 1. The same model is used to train the Density of Space Spectra (DOS) in two different representations, such as discretized representation and a low-dimensional representation of the crystalline materials, by training two models, AE-ALIGNN and D-ALIGNN separately. [16] The derived DOS is helpful in gaining a deeper insight into the electronic properties of the materials and their relationship with ingredient species. For the electronic property prediction, a recent deep learning (DL) model ElemNet is used by leveraging the concept of transfer learning (see the transfer learning architecture in figure [6]). The stability of a compound (by predicting the formation energy) could be successfully determined for both DFT computed dataset and the experimental-based smaller dataset. The model is also applicable in predicting thermal, mechanical, and magnetic properties, which are expensive to calculate experimentally. [17] In a modified version of the ElemNet model, the concept of cross-property deep transfer learning is incorporated for predicting the electronic properties. [18] The Localized Gaussian Process Regression (L-GPR) model that uses a smaller dataset applied to screen the materials based on formation energy. [19] For the same task, Crystal Graph Convolutional Network (CGNN) with slight modification in the convolutional layer has shown improved accuracy compared to DFT-based methods. The modification is done by ignoring the difference in interaction
strength between neighbor nodes in the convolutional layer of the network. The same framework can also predict electrical and physical properties with improved accuracy. In the GBDT model, the relative stability of different materials based on their formation energy and classification task like metal/non-metal based on the acquired bandgap is carried out by Soumya Sanya et al. Another recent model developed by Mohammadreza Karamad et al. is the Orbital Graph Convolutional Neural Network (OGCNN) that uses the orbital field matrix (OFM) descriptor, a data representation method taken from the one-hot vector concept of natural language processing. Here, the representation of an atom is embedded with the orbital-orbital interaction of atoms and the long-range interactions in the local structure. The incorporation of OFM descriptor in the GCNN has improved prediction accuracy for electronic properties like bandgap, Fermi Energy, and Formation energy as compared to state-of-the-art GCNN models. A description of these models is given in detail in Table 2 of Supplementary materials. In the existing SchNet model is extended by including an edge update network because of which the hidden state of receiving atom is responsible for the information interchange among the atoms. This extension improved the accuracy in formation energy prediction. Atom2Vec model is designed for the prediction of the formation energy of elpasolite crystals that are used for radiation detection. The CGCNN and Materials Graph Neural Network (MegNet) are used in predicting magnetic moment and total energy. The DeeperGATGNN is designed using a global attention graph neural network with the inclusion of residual skip connection and differentiable group normalization to allow the network to go deeper. The model showed outstanding performance in bandgap prediction by increasing the hidden layers above 20, whereas other state-of-the-art models tend to crash with more hidden layers. It is also free from overfitting. In addition to property prediction, uncertainty evaluation of ML models in order to determine the trustworthiness of computed data is carried out in [29]. Here three different approaches are used. The first one is the GBDT method with quantile loss function, defined as in equation (1).

\[ L(x^p_i, x_i) = \max[q(x_i, x^p_i), (q - 1) \times (x_i - x^p_i)] \]

where \( q \) is the quantile that gives a value to a group for the observations to fall within that value. \( x^p_i \) is the prediction and \( x_i \) is the outcome. In the second approach, GBDT is used as a base model for the prediction of property, and Gaussian Processes (GP) is used as an error model for finding the prediction intervals. In the third approach, GP is used for determining the uncertainty of the trained model. These models are used for electrical, energetic, mechanical, and optical properties, and the obtained results are compared with each other. The recent progress of ML models has paved the way for solving a basic problem of quantum mechanics: the Schrodinger equation (SE), defined as

\[ H\psi = E\psi \]

The Kernel Ridge Regression Model is used in this task that can establish a non-linear relationship between the atomization energy of a molecule and its characteristic, thereby solving the molecular SE. The trained model is successful in finding new molecular systems with different geometry and composition. The concept of the descriptor 'bag of words, used in natural language processing, performs the encoding of the frequency of a particular word in a text, which is mimicked in the work of Hansen et al. by encoding the interatomic distances in Bag of Bond (BoB) descriptor in the chemical compound space. The model performed well in atomization energy and total energy prediction of molecules. The ALIGNN model in is modified by incorporating the angular information of the atoms in the line graph to get a better atomic structure and is applied for various electronic and molecular properties of the DFT computed dataset.
Figure 1: Two of the mostly used Graph Neural Networks in the literature. 

(a) Schematic of the CGCNN model: The crystal structure is converted to a crystal graph by taking atoms as nodes and atomic bonds as edges from the unit cell. The nodes of the graph go through R convolution layers and L1 hidden layers to produce a resulting graph that considers the local environment of each of the atoms. After the pooling layer, a vector of the whole graph is produced and sent to L2 hidden layer for further processing. The L2 layer then produces the predicted property as output.

(b) Schematic of the ALIGNN model. The graph on the left is the bond graph of a crystal structure. The nodes of the graph are analogous to the atoms, and the edges are analogous to interatomic bonds. From this graph, another graph, L(g) (right), known as the line graph, is derived by considering the edges of the bond graph as nodes and the interatomic bond pair or the triplet of atoms as edges. Message passing is performed between the bond graph and the line graph in the convolution layer.

Molecular properties are also predicted in [33] by Hierarchically Interacting Particle Neural Network (HIP-NN) that uses Linear regression for modeling the local hierarchical energies and Adaptive Moment Estimation (Adam) algorithm for training the model.

For the prediction of dielectric and mechanical properties like Born-effective charge (BEC) tensor, piezoelectric (PZ) tensor, and IR frequency, a research group in [34] have used structural descriptors such as Classical force-field inspired descriptors (CFIDs) and ML models based on gradient-boosting decision tree (GBDT) for both classification and regression task. The regression model yields good accuracy in finding the highest infrared frequency and maximum BEC, whereas the classification models are used for classifying high PZ and dielectric materials. (CFIDs) and (GBDT) are also used to speed up the screening process in predicting magnetic properties of materials. A recently developed model, deeper graph neural networks (deeperGATGNN), that uses ResNet structure and differentiable group normalization in the graph attention layers can learn the relationship between crystal structure and their vibrational energy. The accuracy of the model was suitable for rhombohedral crystals, but it reported high MAE for cubic structures while training on mixed samples revealing the low structural transferability of the model.

1.3 AI in energy material engineering:

A handful of works in energy materials have also been carried out in recent years. Linear regression, Reduced error pruning (REP) tree, Rotation forest+REP tree, and Random subspace+REP tree are explored for predicting band gap of solar cells and metallic glass alloys, giving remarkable accuracy. In this work, a diverse set of descriptors are generated by creating Stoichiometric attributes, electronic structure attributes, elemental property statistics, and Ionic compound attributes. The Gradient Boosting Decision Tree (GBDT) is also used as a binary classification model to find out the promising solar absorber materials by classifying the data based on spectroscopic limited maximum efficiency (SLME) for quick pre-screening of the materials. For screening the high-pressure alloys that are used for hydrogen storage, ML models like RepTree, RFR, and Neural Networks are used. These models are trained to predict the thermodynamic properties, such as hydride enthalpies and entropy of hydrogenation of the alloys. In the same work, low-energy Ti–Mn–Fe structures are detected by predicting the structure and phase with the help of a genetic algorithm. However,
while comparing this structure with DFT and CALPHAD studies, contradictory results are found. In [40], a dataset for LiSi battery materials is designed by finding the random structure relaxations of the material using DFT. The datasets used in the state-of-the-art models are described in table 3 of supplementary materials. For measuring the quantity of dendrite growth in the initiation phase of Li metal anode, ML frameworks have been used recently. [41] In this task, different ML models are used in different phases. In the Isotropic material screening phase, where the stability of electrodeposition is determined for solid electrolytes, the shear and bulk moduli are calculated using the crystal graph convolutional neural network (GC-GCN), and in the second phase, that is, anisotropic material screening, AdaBoost, Lasso, and Bayesian ridge regression are used for prediction of $C_{11}$, $C_{12}$ and $C_{44}$ elastic constants.

The Open Catalyst 2020 (OC20), a DFT-based catalyst dataset, is designed by L Chanussot et al. [42] that contains Transport Equations (BTE) and found that though the convergence time is more in FCNN, it showed good prediction accuracy than prior models[53], Optimization of semiconductor dot devices using ML algorithms[54], supervised ML models in interlayer energy and elastic constant prediction of essential heterostructure for solid and super lubricant materials[55]. Deep Potential Generator (DP-GEN) framework for statistical, mechanical and dynamical properties prediction of Al, Mg and Al-Mg alloys and for the modelling of Potential Energy Surface (PES) using the molecular dynamics (MD) simulation and without inclusion of structural information[56]. 3-D chemical structure prediction using Variational Autoencoder and a 3-D U-Net segmentation network with an attention mechanism[57]. prediction of compounds having highest melting temperature using ordinary least squares regression (OLSR), partial least-squares regression (PLSR), support vector regression (SVR),and Gaussian process regression (GPR) models by preparing separate predictor sets, where first set contains the physical properties and the second one contains both physical and elemental properties[58].
1.4 AI in predicting molecular property:

In molecular property prediction, frameworks like MoleculeNet are designed for predicting four categories of molecular properties: quantum mechanics, physical chemistry, biophysics, and physiology by preparing separate datasets for each of these properties and creating a separate metric and splitting pattern for each of these datasets. Graph Convolutional Networks (GCN) and Graph Isomorphism Networks (GIN) with self-supervised learning mechanisms in order to improve the classification and regression task are used to design the framework Molecular Contrastive Learning of Representations (MoLCLR) for molecular property prediction. The deep tensor neural network (DTNN) designed for quantum chemical property prediction is scalable according to the number of atoms in a molecule. It is capable of predicting data beyond the training set. The DTNN is successfully used in isomer energy prediction, in the classification of molecules based on carbon ring stability, and in some peculiar electronic structure prediction.
The KV-PLM model is capable of learning the co-relation between biomedical text and molecular structures and hence can assist the discovery of the drug. The Schnet model designed to search the chemical space and energy surfaces was successfully used for predicting quantum mechanical property for C_{20} -fullerene, which was not possible with the simulation method. For predicting physicochemical properties from molecular structures, a multiplex graph neural network named Multiplex Molecular Graph Neural Network (MMGNN) is designed and found to be efficient. Beyond the concept of property prediction for some existing materials, an advanced concept in material science is the inverse design framework. Wherein new materials are discovered for a given target property. This is manifested by a deep variational autoencoder neural network with a supervised mechanism called active learning and a generative adversarial deep neural network and have discovered eleven different semiconductor materials and two materials with high bandgap. In , a high-speed inverse design framework named as Fourier-Transformed Crystal Properties (FTCP) for inorganic crystals that can predict the structure and chemistry of a material upon giving some targeted property is designed. The framework is then used for targeted formation energies, bandgap, and for thermoelectric power factor. Conditional GAN (CondGAN) and conditional VAE (CondVAE) models are used to implement the inverse design concept where inorganic compositions are generated from the target property without including the crystal information. Various machine Learning models are also used for engineering new concrete formulas for desirable properties. The realistic samples are generated by conditional distribution $p(y|x)$ so that the properties of the generated data can be controlled by changing the value of $x$. Where $x$ contains the information about strength, age, and environmental impact, and $y$ represents the number of constituent materials. The reduced environmental effect and strength of the formulas are then verified using a regression model by estimating the similarity between generated properties with the desired properties. Some of the tools and frameworks used in implementing DL and ML algorithms in state-of-the-art works are described in table 1.

### Table 1: Tools and Frameworks

| Tools and Frameworks | Description | Link |
|----------------------|-------------|------|
| Scikit-learn         | An Open source easy to use and efficient tool for predictive data analysis | [https://scikit-learn.org/stable/](https://scikit-learn.org/stable/) |
| Tensorflow           | A free and open source library specifically designed for DL models | [https://www.tensorflow.org/](https://www.tensorflow.org/) |
| Theano               | The Python library for DL that can perform fast numerical computations that includes multi-dimensional arrays | [https://pypi.org/project/Theano/](https://pypi.org/project/Theano/) |
| Caffe                | A deep learning framework having an expression architecture that allows the users to switch between CPU and GPU | [https://caffe.berkeleyvision.org/installation.html](https://caffe.berkeleyvision.org/installation.html) |
| MXNet                | It is a fast and scalable DL framework that allows training of fast model and supports multiple programming language. | [https://mxnet.apache.org/versions/1.9.0/](https://mxnet.apache.org/versions/1.9.0/) |
| Keras                | An open source library that acts as an interface for the tensorflow library | [https://keras.io/](https://keras.io/) |
| Pytorch              | Pytorch is a python package that gives two features tensor computation with strong acceleration by GPU and deep neural network built on a automatic differentiation system | [https://pytorch.org/](https://pytorch.org/) |
| CNTK                 | A unified deep learning framework that uses a directed graph and series of computational steps to describe neural network | [https://docs.microsoft.com/en-us/cognitive-toolkit/](https://docs.microsoft.com/en-us/cognitive-toolkit/) |
| PyCaret              | A machine learning framework for automation of machine learning workflows | [https://pycaret.org/](https://pycaret.org/) |
| DeepChem             | A deep learning framework for Drug Discovery, Quantum Chemistry, Materials Science and Biology | [https://deepchem.io/](https://deepchem.io/) |
| Deep Docking         | A deep learning framework for molecular docking | [https://github.com/zhenglz/dockingML](https://github.com/zhenglz/dockingML) |
| MolPAL               | Active learning framework for high throughput virtual screening | [https://github.com/coleygroup/molpal](https://github.com/coleygroup/molpal) |
| Library     | Description                                                                 | URL                                      |
|------------|------------------------------------------------------------------------------|------------------------------------------|
| Hugging face | Machine learning library that creates base model to build on top of TensorFlow and Pytorch | https://huggingface.co/                  |
| GraphInvent | Platform to generate graph based molecules using GNN                         | https://github.com/MolecularAI/GraphINVENT |
| ATOMAI      | Deep learning framework for microscopy data                                 | https://atom.io/packages/ide-python      |
| Veles       | A distributed DL framework                                                   | https://github.com/Samsung/veles         |

2 Important methods:

The recent surge in Artificial Intelligence can be attributed to the availability of datasets and computing power such as Graphics Processing Units, Tensor Processing Units, and other hardware accelerators. These have allowed for the development of intricate and deep structures, which enable for exhaustive investigations such as Material Engineering. In this part, we will go over some of the AI methods used in Material Engineering. To begin, we will review the datasets that are available for AI based material engineering.

2.1 Datasets for material engineering:

Datasets are the fuel of any AI modal. For AI-based material engineering, we need datasets with desired properties and with a sufficient number of samples. Recently, the national institute of standards and technology (NIST) has produced several datasets for material engineering. The JARVIS-DFT is one such dataset. This dataset contains DFT-based material properties of 40000 bulk and 1000 crystalline materials. This dataset contains the properties such as formation energies, bandgaps, elastic, piezoelectric, dielectric constants, magnetic moments, exfoliation energies for van der Waals bonded materials, improved meta-Generalized Gradient Approximations(meta-GGA) bandgaps, frequency-dependent dielectric function, spin-orbit spillage, spectroscopy limited maximum efficiency (SLME), infrared (IR) intensities, electric field gradient (EFG), heterojunction classifications, and Wannier tight-binding Hamiltonians. The next dataset is the Open Quantum Material Database. This dataset is developed and maintained by the Wolverton Research Group at Northwestern University. This dataset contains the thermodynamic and structural properties of 1,022,603 materials.

A detailed list of all the available datasets for AI-based material Engineering is provided in Table 3 of the supplementary document.

2.2 Neural network:

Neural networks are modeled after the biological brain. A neural network consists of three types of layers. These are the input, hidden, and output layers. The input layer is the data feeding layer, the output layer is the final prediction layer and in the hidden layer(s) the feature extraction and computations are executed. Each layer in the network consists of a set of artificial neurons, which are connected to the neurons in the adjacent layers by a set of weights. The weights determine the strength of the connection between two neurons and are the parameters that the network learns during training. The basic operation of a neuron is to take a weighted sum of its inputs, apply an activation function to the result, and pass the output to the neurons in the next layer. The activation function is typically a non-linear function that introduces non-linearity into the network, allowing it to learn complex relationships in the data. A typical Nural Network is as shown in figure 5. Mathematically the forward pass can be derived as $H_i = \sigma (X_i \ast W_i + b_i)$. Where $X_i$ is the input, $W_i$ is the weight matrix, $b_i$ is the bias and $\sigma$ is the activation function, such as sigmoid $\sigma(x) = \frac{1}{1+e^{-x}}$.

The learning process happens by adjusting the weights and biases to achieve the desired output at the output layer. This model can be further deepened by introducing more hidden layers. The deeper the layer the more complex phenomenon can be learned. This type of deep neural network can learn more complex features such as properties of materials. There are few other types of neural network that are extensively used in material engineering. These are Convolutional Neural Network (CNN), Graph Neural Networks (GNNs), Generative model etc.

A convolutional neural network (CNN) is based on the mathematical operation of convolution, which is a way of combining two functions to produce a third function that represents how one of the original functions is modified by the other. In the case of a CNN, the input data (e.g., an image) is convolved with a set of learnable filters to produce a set of feature maps. In the context of a CNN, the input data is typically a 3D tensor with dimensions (width, height, channels), where channels represent the number of color channels (e.g., 3 for RGB images). The filters, or kernels, are also 3D tensors with dimensions (kernel width, kernel height, input channels), where input channels matches the number of channels in the input data. To apply a convolutional layer in a neural network, slide the kernel over the
input data, computing the dot product between the kernel and the local region of the input data at each position. This operation produces a single value, which is used to populate the corresponding position in the output feature map. The mathematical formula for the convolution operation can be expressed in matrix form as follows: 

\[ G = F \ast K \]

where \( F \) is a matrix representation of the input data, \( K \) is a matrix representation of the kernel, and \( G \) is a matrix representation of the output feature map. [71] Zhuo Cao et al. have demonstrated the use of CNN in predicting the properties of crystalline materials. [72] However, performance of CNN generally suffers if the topology is arbitrary or change in orientation of the object. These type of limitations can be avoided using the graph neural network. [73]

2.3 Graph neural networks for efficient material engineering:

Graph Neural Network (GNN) is an artificial neural network that processes and analyzes data structured in graph form. They have grown in popularity due to their capacity to deal with complex associations and dependencies between entities in a graph. Graphs consist of nodes (also known as vertices) and edges that link the nodes. Each node and edge can have connected characteristics, representing properties such as node or edge types, numerical values, or categorical labels. GNNs manipulate a graph by iteratively gathering information from neighboring nodes and edges, using a neural network to change and update the node representations. This process can be repeated over multiple layers, each learning more intricate patterns and dependencies. GNNs have produced positive results in many areas, for instance, recommendation systems, drug discovery, social network analysis, and traffic prediction. They can manage different graphs, such as directed and undirected, bipartite, and heterogeneous graphs. A convenient way to represent molecules is in the form of a graph, where atoms are used to represent the featured nodes, and the interatomic bonds (with bond order) are used to represent edges. Features include properties like atomic identity, formal charge, and aromaticity. [74] These are used in a molecular fingerprint that determines the presence or absence of a substructure in an atom. A typical graph neural network is shown in figure 4.

In GNN based model, interactions between atoms are learned by the atom embedding in a high-dimensional space and updating the embeddings by performing message passing. In recent years, many groundbreaking works have been published in GNN. [32, 15, 49, 25, 46, 28]. In [20], crystal graph is used in property prediction. A similar architecture was applied to predict thermoelectric properties on a dataset of crystal and atomic information. [32] The atomic line graph neural network (ALIGNN) has achieved up to 85% accuracy in solid and molecular property prediction. [15] In [32], the angular information is included explicitly by introducing a line graph. The line graph contains bond distance and bond angle information. The model designed with the inclusion of structural information is trained on crystalline materials properties and on molecular properties that could give good accuracy. This model outperformed conventional descriptors such as CFID. Despite the great potentials of GNN, most of the state-of-the-art GNN models suffers from the issue of over-smoothing where with increasing depth, the model tends to make the embedding of all the nodes similar, which makes it challenging to classify unlabeled node and thus making GNN unscalable. To address this issue, an architecture called Deeper Graph Attention Neural Network (DeeperGATGNN) is introduced. [75]. Before DeeperGATGNN, a simpler version named GATGNN was implemented. It contains two different soft attention layers; the first layer extracts the features at the local level of neighboring atoms. The subsequent attention layer extends this neighborhood-dependent information to the global context. This architecture is then extended by introducing additive skip connections between these soft attention layers and differentiable group normalization (DGN) layers. The DGN makes different clusters of the nodes of a graph, and each cluster is normalized separately, thus having
2.4 Generative models:

"One of the continuing scandals of physical science is that it remains, in general, impossible to predict the structure of even the simplest crystalline solids from a knowledge of their chemical composition," as quoted by John Maddox about 30 years ago. Over the years, though different methods are evolved for crystal structure prediction of molecules and solids, they are computationally expensive, and vast structure space is needed to be searched. As DL algorithms are introduced in this field, Generative Networks(GN), a class of DL algorithms, can tackle this problem to a great extent. GN has the capability of producing samples from a given distribution. The functionality is given as input, and the model outputs a distribution of possible structures. This network works on joint probability distribution \( p(x, y) \), which means they can notice both the molecular representation of a material denoted as \( x \) and its property as \( y \). If the conditional probability is applied, then the notation for design will be \( p(y|x) \), and by reversing the notation, we get \( p(x|y) \), which represents the inverse design of the material. The two most commonly used generative networks are: Variational Autoencoder (VAE) and Generative Adversarial Network (GAN) (see figure 5).

The GAN is extended by adding an extra condition in both generator and discriminator by feeding an input layer \( Y \) to both networks. This extension is Conditional GAN(CGAN). In an attempt to generate chemical compositions of inorganic materials without the crystal structure information, the concept of CGAN is used by Sawada et al. In this model, the popular feature engineering scheme Bag-of-Atoms is used with the additional inclusion of the physical descriptors. In Bag-of-Atoms, the number of atoms in a chemical composition is represented in vector form. The physical descriptors are the fundamental properties of atoms that do not contain crystal information. CGAN is also used for generating new concrete formulas for building materials. In the conditional probability \( p(x|y) \), \( x \) contains the information about strength, age, and environmental impact, and \( y \) represents the number of constituent materials.

2.5 Leveraging transfer learning for improved accuracy:

Needless to say that DL models are data hungry and can give plausible accuracy only after training with millions of data. But experimental datasets are normally smaller compared to computational datasets. The concept of deep transfer learning is therefore embedded in many of the recently developed DL models where knowledge of one model is transferred to another model by making use of the features learned from the huge dataset. To accomplish this, at first, a source model is trained using a large dataset and then model parameters are tweaked by training on target property.

A deeper concept of this is the cross-property deep transfer learning (see figure 6), where the source model and target models are trained for different properties. The properties that don’t have a large dataset can be predicted using this concept. It is implemented by two methods: i) by fine tuning the source model with target data and ii) learning the features from target dataset and then leveraging those in building target model. The Original ElemNet DL model has...
Artificial Intelligence in Material Engineering

Figure 5: Three Generative Models

(a) Schematic of the VAE model: Schematic of a Variational Autoencoder. The encoder acts as a compressor and generates the latent space by mapping the molecules to a vector space which is then mapped back to the molecule representation using the decoder. [1]

(b) Schematic of a Generative Adversarial Network. Two different convolutional neural networks are used in the model. One is used as a generator that generates some pattern from a set of the random input vector, and the discriminator network discriminates whether the data is real data or fakely generated by the model. If the data generated by the generator is labeled as fake by the discriminator, it is backpropagated to the generator. The generator readjusts the weight and resends the improved result to the discriminator, this process continues until it becomes difficult to differentiate between real data and the generator’s data.

(c) The CVAE model is designed for new concrete formulas for building materials

2.6 AI techniques used in traditional analytical instruments:

AI techniques are used extensively and have shown great potential in the existing traditional analytical instruments of MSE, such as X-Ray Diffraction (XRD), TEM, and Scanning Electron Microscopy (SEM) image analysis. In XRD, traditional descriptors that are used for pattern analysis and for mapping the phase diagrams, are found to gone through some significant improvements before implementation of cross property deep transfer learning which results in improved Mean Absolute Error (MAE). The modified version of ElemNet is implemented using TensorFlow 2 (TF2) with Keras as an interface instead of TensorFlow 1. These improvements in the library lead the model to learn chemical interactions and elemental similarities more accurately resulting a reduced in MAE of 0.0405 eV/atom. Again, the use of Monte Carlo Drop out in training, validation and test phases leads to different activation and output for the same input in each run of the model which is a barrier in consistent feature extraction. The model improved its MAE further from 0.0405 eV/atom to 0.0373 eV/atom once this drop out is disabled. These modifications leads to approx 10% improvement in MAE.
be tedious and time-consuming. Recent works made a leap forward through the seamless integration of ML models in depicting compounds of interest and phase diagrams. In [80], a Convolutional Neural Network (CNN) is used for one-to-one identification of XRD spectra of materials processed from an experimental database by removing noise. While comparing the performance of CNN with some other classical ML algorithms, it has shown better results with an accuracy of 96.7%. In [81], a convolutional network and a dense network are used to learn the features of the inference patterns of powdered XRD, which will lead the model to predict the crystal symmetry, which was otherwise done conventionally using some peak finding algorithm. The convolutional network performed well in theoretical data, but it showed poor performance in experimental data, whereas the dense network showed higher classification accuracy for the experimental data. 82% classification accuracy is achieved for the dense network while classifying only half of the samples. At the same time, the CNN could not give good accuracy to be used as in crystal symmetry prediction. In Transmission Electron Microscopy (TEM) also, AI has shown its potential. An unsupervised ML algorithm (Auto detect mNP) has been designed for the classification of particle shapes of metal nanoparticles (mNP) from TEM images. The algorithm can also determine the impurities in mNP synthesis. The algorithm is also able to classify the long rod and short rod nano particles. [82] For automation of structural analysis of nanoparticles from high-resolution TEM (HRTEM) data, a two-stage framework is designed. A CNN with a U-net architecture performs segmentation on HRTEM nanoparticles, and a random forest classifier detects the defects of individual nanoparticle regions with an accuracy of 86%. [51]

2.7 Advantage and disadvantages of AI in material engineering and its future:

The use of AI in material engineering is a dynamic area of research that is evolving continuously. Using the right kind of algorithm can significantly accelerate the discovery of new materials as ML algorithms can learn repetitive patterns, resulting in faster simulation of complex structures and chemical reactions. The challenge of building interatomic potentials is also taken care of by AI-based methods, as the artificial Neural Network has paved the way for the construction of potential energy surfaces with a higher efficiency of several orders of magnitude compared to traditional methods. AI algorithms can also be used for exploring the massive chemical space of a material by training the model with existing samples and then using the trained model for predicting all possible combinations, which was earlier a big hurdle for simulation-based methods such as DFT. Thousands of stable configurations have been discovered by...
researchers by training ML models with the existing datasets. Future researchers can work for more efficient feature space extraction to provide new paradigms for discovering stable material configurations. ML has stepped into the area of drug discovery too. The Graph Neural Networks and other DL models have greatly helped researchers predict the solubility of molecules and drug target interactions for drug material. Another critical area of research in Drug discovery is the prediction of the protein structure of the targeted molecule to make the treatment successful. Here the AI researcher can grab the opportunity and think big for developing ML and DL algorithms to fuel the growth of target protein structure prediction. In energy storage materials, algorithms can be developed to fulfill multiple objectives. For example, properties like dipole orientation, atomic polarization, resonant effect, and relaxation effect are to be predicted simultaneously to screen a dielectric material. These factors may also have inverted coupling relationships to be optimized collaboratively. For optimizing collective properties, single optimization algorithms are not enough. Therefore, in future work, people may go for the development of multi-optimization algorithms. Though ML has revolutionized the discoveries of material science, there are a few challenges that still need to be addressed. The lack of data (especially from experimental results) is one of the significant drawbacks. Again the poor explainability of AI models is another drawback. The complex generative models are generally treated as a black box, where chemical relationships are not firmly established, and the error analysis too is a difficult task. Therefore, the development of both highly accurate and interpretable models will definitely make a leap forward in material science research. The non-viability is a significant hurdle faced by the chemical structures generated by the generative deep learning models. The highly complex chemical structures produced by the generative models outside the existing chemical space are theoretically feasible. However, synthesizing them may not be viable because of the high cost and complexity.

3 Conclusion:

In conclusion, AI will radically change the ways of developing materials. This will help us to find the materials of desired properties efficiently. This will reduce the time, money, and effort that are needed to create a material. The capabilities of traditional analytical tools will also be improved by adopting the advantages of AI and ML. Recently applied graph neural network-based approaches and generative adversarial algorithms are helping in the rapid development of drugs. The Google Alpha Fold is one such example, which helps us to find the folding of proteins with very high accuracy and thereby find appropriate molecules for drugs. Again various computer vision-based tools are helping us to analyze traditional analytical tools such as transmission electron microscopy (TEM), scanning electron microscope (SEM), Atomic Force Microscopy (AFM), etc. The traditional computation tools such as DFT and in-silico methods are also defeated by AI and ML-based algorithms, both in terms of accuracy and efficiency. All these development have brought us the hope to engineer materials that can meet the demands and also shape the future.

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Note: The supplementary is available at the end of the reference section

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### Supplementary Tables

Table 2: The first column of the table contains some of the latest AI, ML and DL models used for materials property prediction, second column indicating the type of property being predicted, third column gives the details of the predicted property, fourth column gives the performance of the respective models in different parameters and the final column categorises the model based on the techniques of that model.

| Model Type | Property Type | Properties to Predict | Accuracy/Performance | Models based on Techniques |
|------------|---------------|-----------------------|----------------------|---------------------------|
| Active Learning + Roost + MatGNN | Inverse Design | To discover new stable Materials and Semiconductor | discovered one high bandgap material and six semiconductor in a specified range | Generative model + Generative adversarial network |
| ALIGNN | Electronic | | | Graph Neural Network |
| CGCNN | Electronic/ Elastic | | | GNN |

**Model Type:** Active Learning + Roost + MatGNN

**Property Type:** Inverse Design

**Properties to Predict:**
- Bandgap (MP dataset)
- Formation Energy (MP dataset)
- Bandgap (JARVIS-DFT dataset)
- Formation Energy (JARVIS-DFT dataset)
- Total energy
- Ehull
- Bandgap (MBJ)
- Voigt bulk
- shear modulus
- Magnetic Moment
- Spectroscopic Limited Maximum Efficiency
- Spillage
- Kpoint-length
- Plane-wave cutoff
- $\epsilon_x$ (OPT)
- $\epsilon_y$ (OPT)
- $\epsilon_z$ (OPT)
- $\epsilon_x$ (MBJ)
- $\epsilon_y$ (MBJ)
- $\epsilon_z$ (MBJ)
- $\epsilon$ (DBPT: elec-ionic)
- Max. piezoelectric strain coeff (dij)
- Max. piezo. stress coeff (eij)
- Exfoliation Energy
- Max. EFG
- avg. me
- avg.mh
- n-Seebeck
- n-PF
- P-Seebeck
- p-PF
- Formation energy
- Absolute Energy
- Bandgap
- Fermi Energy

**Accuracy/Performance:**
- 0.022 eV/atom
- 0.218 eV
- 0.033 eV/atom
- 0.14 eV
- 0.037 eV/atom
- 0.076 eV
- 0.31 eV
- 10.40 GPa
- 9.48 GPa
- 0.26 µB
- 4.52 No unit
- 0.35 No unit
- 9.51 Å
- 133.8 eV
- 20.40 No unit
- 19.99 No unit
- 19.57 No unit
- 24.05 No unit
- 23.65 No unit
- 23.73 No unit
- 28.15 No unit
- 20.57 CN−1
- 0.147 cm−2
- 51.42 meV (atom)−1
- 19.12 1021 V m−2
- 0.085 electron mass unit
- 0.124 electron mass unit
- 40.92 μVK−1
- 442.3 μW (mK)−2
- 42.42 μVK−1
- 440.26 μW (mK)−2
- 0.039 eV/atom
- 0.072 eV/atom
- 0.388 eV
- 0.363 eV

**Models based on Techniques:**
- Generative model + Generative adversarial network
- Graph Neural Network
- GNN
Continuation of Table 2

| Classification | Bulk modulus | Shear modulus | Poisson ratio |
|----------------|--------------|---------------|---------------|
| of metal       | 0.054 log(Gpa) | 0.087 log(Gpa) | 0.030 log(Gpa) |
| for threshold 0.5 | 0.8          | 0.8           | 0.95          |

| Classification | Global warming Potential (GWP) | Acidification Potential (AP) | Strength Predictor Performance |
|----------------|--------------------------------|-----------------------------|-------------------------------|
| (of the formulas) | MAE 7.187 | RMSE 9.374 | MAE 4.457 (>90 days) |
|                 | R2 0.979   |               | R2 0.974                  |
|                 | RMSE 0.019 |               | RMSE 0.125 (>90 days)    |
|                 | R2 0.974   |               | R2 0.789 (>90 days)      |

| Methodology | Technique | Application | Performance Measures |
|-------------|-----------|-------------|-----------------------|
| Conditional Variational Autoencoder (CVAE) | To design concrete formulas | 99% Segment the locations of molecules | MAE 0.127 |
|                     |           | 90% Reconstruction | MAE 0.348  |
|                     |           | 66% Classification of Species | MAE 0.092  |
|                     |           | 65.40% Nearest Atom Species Prediction | MAE 0.068 |
| CVAE + 3-D U-Net segmentation model | Encode and Decode 3-D atomic position and species | 99% for Single Unit cell | MAE 0.338 |
|                     |           | 90% for Repeating Unit cell | MAE 0.5012 |
| Compositionally Restricted Attention-based Network (CrabNet) | Electronic Thermal Elastic | 99% Castelli perovskites | MAE 0.263 |
|                     |           | 90% Refractive Index | MAE 0.341 |
|                     |           | 66% Shear modulus | MAE 0.092 |
|                     |           | 65.40% Bulk Modulus | MAE 0.068 |
|                     |           | 99% Experimental band gap | MAE 0.338 |
|                     |           | 90% Exfoliation Energy | MAE 0.5012 |

| Methodology | Technique | Application | Performance Measures |
|-------------|-----------|-------------|-----------------------|
| Bartel Decomposition | | | MAE 0.093 |
| Bartel Formation | | | MAE 0.063 |
| MP bulk modulus | | | MAE 0.059 |
| MP Elastic anisotropy | | | MAE 11.209 |
| MP Energy above convex hull | | | MAE 8.263 |
| MP Magnetic Moment | | | MAE 0.089 |
| MP shear modulus | | | MAE 2.105 |
| OQMD Band gap | | | MAE 12.787 |
| OQMD Energy per Atom | | | MAE 0.049 |
| | | | MAE 0.033 |
## Continuation of Table 2

| Method                              | Property                      | Crystal state | Elastic | Band Gap (for Zn based systems) | Band Gap (for Cu based systems) | Band Gap (for Mg based systems) | MAE                      | Graph Convolutional Neural Network (GCNN) |
|-------------------------------------|-------------------------------|---------------|---------|----------------------------------|----------------------------------|----------------------------------|--------------------------|-------------------------------------------|
| OQMD Formation Enthalpy            |                               |               |         |                                  |                                  |                                 | 0.031                    |                                           |
| OQMD Volume per atom               |                               |               |         |                                  |                                  |                                 | 0.277                    |                                           |
| Crystal eXplainable Property Predictor (CrysXPP) [84] |                               |               |         |                                  |                                  |                                 | 0.086 ev/atom             |                                           |
|                                    |                               |               |         | 0.467 ev                          |                                  |                                 | 0.08 log(Gpa)             |                                           |
|                                    |                               |               |         | 0.471 ev                          |                                  |                                 | 0.105 log(Gpa)            |                                           |
|                                    |                               |               |         | 0.035 log(Gpa)                    |                                  |                                 | 0.1903 ev                 |                                           |
|                                    |                               |               |         | 1.4995 ev                         |                                  |                                 | 1.4995 ev                 |                                           |
| Deep Adaptive Regressive Weighted Intelligent Network (DARWIN) [27] |                               |               |         |                                  |                                  |                                 | 34.97% ev/atom            |                                           |
| DeeperGATGNN [28]                  | Physico-Chemical              |               |         |                                  |                                  |                                 | 29.55%                   |                                           |
|                                    |                               |               |         |                                  |                                  |                                 | 14.03%                   |                                           |
|                                    |                               |               |         |                                  |                                  |                                 | 15.76%                   |                                           |
|                                    |                               |               |         |                                  |                                  |                                 | 5.34%                    |                                           |
|                                    |                               |               |         |                                  |                                  |                                 | 5.42%                    |                                           |
| (DimeNet++) [85]                   | Thermodynamic, Electronic     |               |         | Dipole Moment (mu)                |                                  |                                 | 0.0297 D                 |                                           |
|                                    |                               |               |         | Electronic Polarizability (alpha) |                                  |                                 | 0.0435a03                |                                           |
|                                    |                               |               |         | HOMO                             |                                  |                                 | 24.6meV                  |                                           |
|                                    |                               |               |         | LUMO                             |                                  |                                 | 19.5                     |                                           |
|                                    |                               |               |         | Energy difference of HOMO and LUMO |                                  |                                 | 32.6meV                  |                                           |
|                                    |                               |               |         | electronic spatial extent <R2>    |                                  |                                 | 0.331a02                 |                                           |
|                                    |                               |               |         | ZPVE                             |                                  |                                 | 1.21meV                  |                                           |
|                                    |                               |               |         | Internal Energy at 0k (U0)        |                                  |                                 | 6.32meV                  |                                           |
|                                    |                               |               |         | Internal Energy at 298K (U)       |                                  |                                 | 6.28meV                  |                                           |
|                                    |                               |               |         | enthalpy at 298 K(H)              |                                  |                                 | 6.53meV                  |                                           |
|                                    |                               |               |         | Gibbs free energy at 298 K(G),    |                                  |                                 | 7.56meV                  |                                           |
|                                    |                               |               |         | heat capacity at 298 K (Cv)       |                                  |                                 | 0.0230cal/mol K          |                                           |
| Decision-Trees (DT) [38]           | Classification Task          |               |         | Classify materials based on spectroscopic limited maximum efficiency (SLME) |                                  |                                 | 0.67                     | Classification Model                      |
| randomforest (RF) [38]             |                               |               |         |                                  |                                  |                                 | 0.79                     |                                           |
| K-nearest neighbor (KNN) [38]       |                               |               |         |                                  |                                  |                                 | 0.77                     |                                           |
| Multi-layer perceptron (MLP) [38]  |                               |               |         |                                  |                                  |                                 | 0.8                      |                                           |

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| Method                                     | Task                                      | MAE (training size=50k) | R2 (training size=50k) |
|-------------------------------------------|-------------------------------------------|--------------------------|------------------------|
| GBDT in scikit learn (SK-GB) [38]         | Electronic Formation Enthalpy             | 0.050 ± 0.0007 ev/atom  |            |
| GBDT in XGBoost (XGB) [38]                | Electronic Formation Enthalpy             | 0.050 ± 0.0007 ev/atom  |            |
| GBDT in LightGBM (LGB) [38]              | Electronic Formation Enthalpy             | 0.050 ± 0.0007 ev/atom  |            |
| ElemNet [86]                              | Electronic Formation Enthalpy             | 0.050 ± 0.0007 ev/atom  |            |
| Fully Connected Neural Network (FCNN) [87]| Electronic Formation Energy               | 0.160 ev                 | 0.93       |
| Heuristic and Ensemble of decision trees  | Electronic Formation Enthalpy             | 0.120 ev                 | 0.95       |
| Hierarchically Interacting Particle Neural Network (HIP-NN) [33] | Energy of Benzene, Energy of Malonaldehyde, Energy of Salicylic Acid, Energy of Toluene | H= 7.54e−3 ± 8.70e−4 C= 6.77e−3 ± 3.59e−4 M= 04e−2 ± 4.94e−4 1 |          |
| Hydra-GNN [48]                            | Multi-task Learning (MTL), Mixing Enthalpy (H), Charge transfer (C), Magnetic Moment (M) | H= 7.54e−3 ± 8.70e−4 C= 6.77e−3 ± 3.59e−4 M= 04e−2 ± 4.94e−4 1 |          |
| IRNET [89]                                | Electronic and Elemental OQMD-C Formation Enthalpy | 0.054                   |            |
|                                          | OQMD-C Bandgap                           | 0.051                   |            |
|                                          | OQMD-C Energy per atom                   | 0.0696                  |            |
|                                          | OQMD-C Volume per atom                   | 0.415                   |            |
|                                          | MP-C Bandgap                             | 0.363                   |            |
|                                          | MP-C density                             | 0.348                   |            |
|                                          | MP-C Energy-above-hull                   | 0.091                   |            |
|                                          | MP-C Energy-per-atom                     | 0.143                   |            |
|                                          | MP-C Total magnetization                 | 3.005                   |            |
|                                          | MP-C Volume                              | 215.037                 |            |

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| Method | Task | Description | MAE (avg) | Improvement over CGCNN |
|--------|------|-------------|----------|------------------------|
| JARVIS-STMnet [12] | Classification Task | Classification of five lattice classes (square, hexagon, rhombus/centered-rectangle, rectangle and parallelogram/oblique) | 0.9 | | Convolutional Neural Network (CNN) |
| MATGNN [90] | Inverse design | Generates hypothetical inorganic materials | 84.5% chemically valid samples out of total generated samples | | Generative adversarial network |
| Message Passing Neural Network (MPNN)(enn-s2s) [91] | Chemical Property | mu, alpha, HOMO, LUMO, Gap, R2, ZPVE, U0, U, H, G, Cv, Omega, | MAE(avg) 0.68 | GNN |
| MPNN (enn-s2s-ens5) [91] | Quantum mechanical, physical chemistry, biophysical affinity, physiological | Properties on QM7 dataset | MAE (on best model) DTNN: 8.75 | | Different Variations of GNN |
| Moleculenet [59] | Quantum Chemical | Properties on QM7b dataset | MAE DTNN: 1.77a | | |
| | | Properties on QM8 dataset | MAE MPNN: 0.0143 | | |
| | | Properties on QM9 dataset | MAE DTNN: 2.35 | | |
| | | Properties on ESOL | MAE MPNN: 0.58 | | |
| | | Properties on FreeSolv | MAE MPNN: 1.15 | | |
| | | Properties on Lipophilicity | RMSE GC: 0.655 | | |
| | | Properties on PCBA | AUC-PRC GC: 0.136 | | |
| | | Properties on MUV | AUC-PRC Weave: 0.109 | | |
| | | Properties on HIV | AUC-PRC GC: 0.763 | | |
| | | Properties on BACE | AUC-PRC Weave: 0.806 | | |
| | | Properties on PDBBind(FULL) | RMSE GC: 1.44 | | |
| | | Properties on BBBP | AUC-PRC GC: 0.690 | | |
| | | Properties on Tox21 | AUC-PRC GC: 0.829 | | |
| | | Properties on ToxCast | AUC-PRC Weave: 0.742 | | |
| | | Properties on SIDER | AUC-PRC GC: 0.638 | | |
| | | Properties on ClinTox | AUC-PRC Weave: 0.832 | | |
| Multiplex Molecular Graph Neural Network (MXMNet) with batch size(BS) =128 and cut off distance dg [64] | Quantum Chemical | mu, alpha, HOMO, LUMO, Gap, R2, ZPVE, U0, U, H, G, Cv, Omega, | MAE(avg) 0.92% | GNN |
| MT-CGCNN [21] | Electronic | Multi-task Learning (Formation Energy and Bandgap) | Improvement over CGCNN 8.30% | GNN |
| | | (Formation Energy and Fermi Energy) | 3.80% | |
| | | (Bandgap and Fermi Energy) | 1.70% | |
## Continuation of Table 2

| Method | Task | Metric | Value |
|--------|------|--------|-------|
| Orbital Graph Convolutional Neural Network (OGCNN) [22] | Electrical | Formation Energy, Bandgap, Fermi Energy | 4.40% |
| | | Lanthanides-formation energy | MAE | 0.06 ev/atom |
| | | Perovskites-formation energy | MAE | 0.05 ev/atom |
| | | MP-formation energy | MAE | 0.03 ev/atom |
| | | MP-Band Gap | MAE | 0.032 ev |
| | | MP-Fermi Energy | MAE | 0.38 ev |
| OrbNet [92] | Quantum Mechanical | Total Energy for Molecules and Relative Conformer Energy for Molecules | 33% (improvement over best prior model) Similar accuracy as DFT method |
| Roost [Ensemble] [93] | Electronic | Bandgap | MAE | 0.0241 ev |
| | | | RMSE | 0.0871 ev |
| SOAP + SchNet Model [94] | Electronic | Bandgap | MAE | 0.388 ev |
| UNet+proto-DenseNet [95] | To find refined pattern | | | 80.05% |

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| Category                          | Database Name                          | Description                                                                 | Link                                                                 |
|----------------------------------|----------------------------------------|-----------------------------------------------------------------------------|----------------------------------------------------------------------|
| Quantum Physical                 | JARVIS-DFT 3D [34]                     | The database contains electrical, magnetic and electro-magnetic properties of 40000 bulk and 1000 low-dimensional crystalline materials | https://www.nist.gov/programs-projects/jarvis-dft                   |
| Structural                       | Open Quantum Materials Database (OQMD) [34] | Contains thermodynamic and structural properties of 1,022,603 materials        | https://oqmd.org/                                                   |
| Mechanical and Thermal           | (AFLOWLIB) [35]                        | The database consists of 3,528,653 material compounds with over 733,959,824 electric, elastic and thermal properties | http://www.aflowlib.org/                                          |
| Chemical                         | Zinc [94]                              | A collection of commercially available chemical compounds prepared for virtual screening | https://zinc12.docking.org/                                         |
| Crystallo-graphic                | Inorganic Crystal Structure Database (ICSD) [78] | Contains 262242 crystal structures of elements to Quaternary compounds as of May 2022 | https://icsd-products.fiz-karlsruhe.de/                             |
| Structural                       | NOMAD [79]                             | Contains ab initio electronic-structure data from DFT and other methods      | https://nomad-lab.eu/index.php?page=repo-arch                      |
| Computational Chemistry          | ioChem-BD [4]                          | A digital repository that deals with computational chemistry dataset     | https://www.iochem-bd.org/                                        |
| Multivariate                     | Materials Experiment and Analysis Database (MEAD) [78] | Contains raw and metadata obtained from material synthesis and characterization experiments also contains the property and performance analysis of that data. | https://solartfuelshub.org/materials-experiment-and-analysis-database |
| Multivariate                     | UCI Machine Learning Repository [68]   | Is a collection of over 550 datasets                                      | https://paperswithcode.com/dataset/ucimachine-learning-repository  |
| Structural and surface morphology| Crystallium [9]                        | Contains surface properties of 145 crystals of 74 elements available and Grain Boundary properties of 58 crystals of 58 elements | http://crystallium.materialsvirtuallab.org/                         |
| Quantum Physical                 | Materials Project(MP) [32]             | It is consist of inorganic compounds, band structures, molecules, nano porous materials and their properties like Magnetic moment, formation energy, energy above hull etc. | https://materialsproject.org                                        |
| Structural                       | Crystallography Open Database (COD) [38] | an Open-access database containing crystal structures of organic, inorganic, metal-organic compounds and minerals | http://www.crystallography.net/cod/                                |
| Thermo-dynamics                  | SGTE Solid Substance (SSUB) [17]       | contains thermochemical property for about 4300 condensed or gaseous species | https://www.sgte.net/en/neu                                        |
| Quantum Chemistry                | QMOF [96]                              | Contains quantum-chemical properties of MOF                                | https://github.com/arosen93/QMOF                                   |
| Metal–organic framework          | Reduced_HMOF [96]                      | Contains 51,163 unique hypothetical MOFs with genetic information          | https://mof.tech.northwestern.edu/                                 |
| Metal–organic framework          | CoRE MOF-2019 [97]                     | Contains 3D porous MOFs that are directly usable in molecular simulations or electronic structure calculations | https://zenodo.org/record/3370144-#.Yr3UBnZBzIU                     |
| Energy Material                  | Hydrogen Storage Materials Database [39] | It contains 2722 hydrogen storage materials with their composition and hydrogen gravimetric capacity | http://surl.li/cejcd                                              |
| Artificial Intelligence in Material Engineering |
|-----------------------------------------------|
| **Structural and Quantum Mechanical** Database |
| Structural and Quantum Mechanical Database [59] |
| Contains one million 3-D structural data of molecules |
| https://www.ccdc.cam.ac.uk/solutions/csd-core/components/csd/ |
| Structural and Quantum Mechanical Database [59] |
| Contains properties of Polymer, Inorganic and Metallic materials and computational electronic structures of materials |
| https://mits.nims.go.jp/en/ |
| Quantum Chemistry QM7 [59] |
| A subset of GDB-13 dataset containing 7165 molecules |
| http://quantum-machine.org/datasets/ |
| Quantum Chemistry QM7b [59] |
| An extension of QM7 dataset by predicting 13 additional properties. |
| http://quantum-machine.org/datasets/ |
| Quantum Chemistry QM8 [59] |
| Contains electronic spectra and excited space energy of small molecules |
| https://moleculenet.org/datasets-1 |
| Quantum Chemistry QM9 [99] |
| Gives Quantum Chemical Properties of small organic molecules |
| http://quantum-machine.org/datasets/ |
| Quantum Chemistry Free Solvation Database (FreeSolv) [59] |
| Contains hydration free energy of experimental and calculated water solubility data |
| https://github.com/MobleyLab/FreeSolv |
| Quantum Chemistry ESOL [59] |
| Solubility database of 1128 compounds |
| https://integbio.jp/dbcatalog/en/record/nbdc00440 |
| Quantum Chemistry Organic Materials Database (OMDB) [94] |
| Contains electronic properties of organic crystal structures |
| https://omdb.mathub.io/dataset. |
| XRD DiffraNet [80] |
| Contains 25,000 labeled serial crystallography diffraction images. |
| https://arturluis.github.io/diffranet/ |
| Molecular PubChem [59] |
| Contains chemical molecules and their activities against biological assays |
| https://pubchem.ncbi.nlm.nih.gov/ |
| Quantum physical OC20 [42] |
| Contains 1,281,040 DFT relaxations for materials, surfaces and adsorbates and their molecular dynamics, randomly perturbed and electronic structure analyses. |
| https://github.com/Open-Catalyst-Project/ocp/blob/main/DATASET.md |
| Structural and Surface morphology Warwick Electron Microscopy Datasets [82] |
| Contains 19769 experimental scanning transmission electron microscopy2 (STEM) images, 17266 experimental transmission electron microscopy2 (TEM) images and 98340 simulated TEM exit wavefunctions in three different datasets. |
| https://github.com/Jeffrey-Ede/datasets |
| Solid-state physics and Synthesis Text-mined dataset of inorganic materials synthesis recipes [50] |
| Contains 19,488 synthesis entries from 53,538 solid-state synthesis paragraphs that uses using text mining and natural language processing approaches |
| https://figshare.com/articles/dataset/solid-state_dataset_2019-06-27_upd_json/9722159/3 |
| Molecular GDB database [59] |
| Contains small organic molecules up to 13 atoms of C, N, O, S and Cl based on simple chemical stability and synthetic feasibility rules |
| https://pubs.acs.org/doi/10.1021/ci600423u |
| Structural and physical Concrete Compressive Strength [59] |
| A multivariate dataset containing concrete compressive strength (MPa) for a given mixture for a particular time was determined from laboratory. |
| http://surl.li/cejcc |
| Physiology and molecular medicine Clintox [59] |
| For a total of 1491 drug compounds, clinical trial toxicity (or absence of toxicity) FDA approval status are included. |
| https://lifesci.dgl.ai/api/data.html |
| Molecular LIT-PCBA [100] |
| From PubChem dataset, 149 dose-response bioassays are included by removing false positives and assay artifacts but keepings active and inactive compounds having similar molecular property. |
| https://drugdesign.unistra.fr/LIT-PCBA/ |
| Bio Molecular          | PDBBind database [59] | Contains 23496 biomolecular complexes with their binding affinity data | http://www.pdbbind.org.cn/ |
|-----------------------|------------------------|---------------------------------------------------------------------|----------------------------|
| **Reactions**         | Reaxys database [101]  | It contains organic and organometallic reactions                    | https://www.reaxys.com/#/   |
| **Structural and Surface morphology** | JARVIS_STM [12] | Contains scanning tunneling microscope (STM) images | https://jarvis.nist.gov/login?next=/jarvisstm |
| Structural            | Database of Wannier tight binding Hamiltonians (WTBH) | Electronic band structure calculations of WTBH | https://github.com/usnistgov/jarvis |
| Chemical              | InfoChem [9]           | Contains large number of known reactions and molecules             | https://www.deepmatter.io/about-us/infochem |
| Chemical              | Citrination [45]       | An experimental based dataset containing chemical information of materials | https://citrination.com/datasets |
| Physical Chemistry    | Lipophilicity [100]    | Contains chemical structure (SMILES) of 1,130 organic compounds and their n-octanol/buffer solution distribution coefficients at pH 7.4 | https://deepai.org/dataset/lipophilicity |
| BioPhysics            | Maximum Unbiased Validation (MUV) [59] | A dataset selected from PubChem BioAssay that contains 17 different tasks of 90 thousand compounds | https://www.tubraunschweig.de/en/pharmchem/forschung/baumann/translate-to-english-muv |
| BioPhysics            | HIV [59]               | Contains 40000 compounds that have the ability to inhibit HIV replication | https://data.unicef.org/resources/dataset/hiv-aids-statistical-tables/ |
| Physiology            | The Blood–brain barrier penetration (BBBP) [59] | A blood-brain barrier dataset for prediction of barrier permeability | https://github.com/theochem/B3DB |
| BioPhysics            | BACE [59]              | Provides binding results for human β-secretase 1 inhibitors         | https://enamine.net/compound-libraries/targeted-libraries/bace-library |
| Physiology            | Tox21 [59]             | Measures toxicity of 8014 compounds                                 | https://paperswithcode.com/dataset/tox21-1 |
| Physiology            | ToxCast [59]            | Contains toxicity of compounds for and larger in size as compared to Tox21 | https://tox21.gov/data-and-tools/ |
| Physiology            | Cider [59]             | Contains market drugs and their adverse reactions                   | http://sideeffects.embl.de/ |
| Molecular Dynamics    | COLL Dataset [85]      | Contains Molecular Collision configurations                        | https://figshare.com/articles/dataset/COLL_Dataset_v1_2/13289165/1 |
| Crystallography and Spectroscopy | RRUFF [103] | Contains Raman spectra, X-ray diffraction & chemistry data for minerals | https://rruff.info/ |
| Chemical              | Melting Point Dataset [104] | Contains melting point of around 8000 chemical structures.         | https://old.datahub.io/dataset/open-melting-point-data |
| Multivariate          | Superconductivity Dataset [104] | Contains Chemical Formula and relevant features of about 21263 superconductors. | https://archive.ics.uci.edu/ml/datasets/superconductivity+data |
| Thermoelectric        | UCSB Thermoelectrics dataset [104] | The database contains Electrical conductivity, Power factor and Seebeck coefficient of thermoelectric materials | https://citrination.com/datasets/150557/show_files |
| Electronic            | dataset of Strehlow and Cook [104] | Contains energy bandgaps of semiconductors and Insulators | https://srdf.nist.gov/jpcrdreprint/1.3253115.pdf |
| Material Type               | Reference | Model/Framework Name                          | Description                                                                                                                                                                                                 |
|----------------------------|-----------|-----------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Inorganic Materials        | [66]      | Fourier Transformed Crystal Properties (FTCP) | The model is used to predict the structure and chemistry of inorganic crystals for some targeted property                                                                                                   |
|                            | [46]      | Modified CGCNN                                | Local energy prediction of inorganic materials is performed using Graph Neural Network                                                                                                                      |
|                            | [81]      | Convolutional Neural Network + Deep Dense Network | Artificial Intelligence based prediction of Space Group Determination problem for powdered XRD pattern of inorganic non-magnetic materials is carried out.                                                   |
|                            | [46]      | CGCNN                                         | CGCNN model is used in inorganic crystals of different compositions and different structures for finding elemental and local environment similarities                                                                 |
|                            | [67]      | Conditional GAN and Conditional VAE           | Inverse design framework is used to generate inorganic compositions from desired property, without crystal structure information                                                                            |
|                            | [14]      | Random Forest                                | Random Forest ML algorithms are used for finding critical temperature of inorganic crystals                                                                                                                   |
|                            | [50]      | Artificial Neural Network and Gaussian Processes | For finding a relationship between reaction condition and resulting spectra of inorganic nano particles, Artificial Neural Network and Gaussian Processes have been used.                                          |
|                            | [90]      | Generative Machine Learning Model (MatGAN)    | A GAN is developed for learning the chemical compositions of inorganic materials                                                                                                                             |
|                            | [89]      | IRNET                                         | Residual connection is used for predicting formation enthalpy of inorganic materials                                                                                                                        |
|                            | [87]      | ORGANIC                                      | A framework named as ORGANIC, which is an Objective-reinforced Generative model is designed and applied in organic photovoltaic materials.                                                                     |
|                            | [15]      | ALIGNN                                       | The ALIGNN Model is applied in Metal-Organic Framework (MOF) materials to screen the MOFs that help in reduction of CO2                                                                                     |
|                            | [96]      | Gaussian Process Regression, Support Vector Regression, Neural Network | Different ML approaches are explored to find out the relationship of structure of MOF and their methane uptake                                                                                             |
|                            | [44]      | Preffered Potential (PFP)                    | A neural network potential is developed and applied in MOF for molecular adsorption                                                                                                                          |
|                            | [92]      | Gaussian Process Regression (GPR)             | An uncertainty prediction scheme for ML models is developed and tested in chemical shielding of H NMR in organic crystals and formation energy prediction of small organic molecules.                             |
|                            | [105]     | SOAP model with kernel ridge regression and Schnet | SOAP kernel and SchNet models are used for bandgap prediction of crystal structures of Large Organic molecules                                                                                             |
|                            | [106]     | Multi-task Deep Artificial Neural Network      | ML model is used for prediction of electronic ground state property and excited state properties of organic molecules                                                                                       |
|                            | [107]     | ChemMIxNet                                    | ChemMIxNet model is developed and applied on water solubility dataset of small organic molecules                                                                                                           |
|                            | [107]     | ChemMIxNet                                    | A ML Model CheMIxNet is used to predict HOMO value of Organic photovoltaic cells                                                                                                                          |
| Organic Materials          | [40]      | MegNet                                        | Designed a GNN named as MegNet to compute the atomic force and stress tensor of unit cell of battery materials.                                                                                           |
| Energy Storage Materials   |           |                                               |                                                                                                                                                                                                             |
| Page | Description |
|------|-------------|
| 38   | Gradient Boosting Decision Tree (GBDT) ML models are used for classifying solar absorber materials based on spectroscopic limited maximum efficiency (SLME) |
| 37   | Linear Regression, Reduced Error Pruning (REP) tree, Rotation forest+REP tree, Random Subspace+REP tree ML model is designed for Bandgap prediction of solar cell materials |
| 39   | Rep Tree, Random Forest Regression and Neural Networks ML framework is used for predicting high pressure alloys that can store hydrogen. |
| 108  | Convolutional Neural Network CN model is used to recognize mixed dimensional (2D-0D) Formamidinium Bismuth Iodides as they are useful in energy consumption |
| 42   | CGCNN, Schnet, Dimenet++ Different state-of-the art Graph Neural Networks are applied on a catalyst dataset. |
| 109  | Artificial Neural Network as classifier and calculator Neural Networks are used for lithium-ion battery design that can reduce the computational time by orders of magnitude. |
| 107  | ChemMIxNet CheMixNet model is applied on the compounds that has the ability to slow down HIV replication in vitro study |
| 59   | Moleculenet The ML framework Moleculenet is designed and used on properties of drug molecules. |
| 110  | Densenet A generative model ,Densenet is used to design de Novo drug. |
| 62   | KV-PLM The model named KV-PLM is designed to assist in the discovery of drug. |
| 111  | OrbNet The deep learning model Orbnet is designed and applied in drug dataset that showed prediction accuracy same as DFT with reduced computational cost. |
| 112  | Random Forest Classifier Random Forest classifier is used for segmenting polymer blends that are used for pharmaceutical tablets. |
| 113  | K-nearest neighbour, support vector machine (SVM), ANN ML algorithms are used for phase selection of High Entropy Alloys (HEA) that is used for medical implant |
| 114  | Linear Regression, polynomial Regression model, SVM with three different kernel functions, regression tree model, k-nearest neighbour model, and ANN with backpropagation Employed ML surrogate models combined with experimental methods for finding High Entropy Alloy (HEA) for targeted property. |
| 115  | Nine different Classification Models With the help of a Genetic algorithm, suitable ML model and descriptors are selected for Phase classification of HEA |
| 116  | Decision Tree Decision tree classifiers are used for analysing Cytotoxicity of nano-particles based on cell viability |
| 117  | Linear Model, Non-linear Model and Convolutional Neural Network (CNN) ML algorithms are employed on biological composites to explore the mechanical properties |
| 118  | Random Forest ensembled with Additive Regression (RF_AR) Ensemble methods are used in designing bio glass |
| 119  | Support Vector Machine Support Vector Machine is used for screening the dielectric polymers |
| 120  | ANN models surrogate models are used for surface properties such as protein adsorption prediction and cellular response for biodegradable polymers. |

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Biography

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