INTRODUCTION

Machine learning tries to generate statistical models for data analysis and prediction using learning algorithms. Without having been particularly designed for a given task, the ML algorithms ought to be able to train on their own (depending on the presented data) and produce accurate predictions. Beyond theoretical improvements, machine learning applications have advanced quickly in recent years, thanks to the work of academics from a variety of professions, including computer scientists and experts in the creation of AI algorithms. Chemical and materials sciences have been impacted by the use of machine learning to speed up particular computing operations or to tackle issues for which conventional modeling approaches were inadequate, among many other disciplines of inquiry. One can create a model for analysing materials if they have enough data in the right format. Choosing the right algorithms, learning from training data, and producing precise predictions are all steps in the modeling process.

ABSTRACT

Over the past ten years, the rate of systematic materials discovery has accelerated. Studies that systematically examine different families of materials with the intention of finding existing materials with unknown qualities or developing new materials with desired properties are multiplying at a startling rate. In terms of computation, molecular simulations have become more sophisticated, enabling researchers to predict the structure and characteristics of complex materials even before they are ever created. High-throughput screening methods can be used with chemical characteristics prediction to aid in the discovery of novel materials. Due to their promising capacities to extract and make use of data-driven information, applications of artificial intelligence, machine learning, and deep learning techniques in the field of materials science are becoming more widespread. Given the composition of the material, we use predictive models for a range of material attributes to help with this procedure. Multiple databases are used to compile the input data necessary to train the machine learning model. Once trained, it can be used to apply predictions for various input data.

LITERATURE REVIEW

Machine Learning in Material Science:

This paper not only outlines the fundamental operational steps in machine learning's analysis of the material properties, but also summarizes recent applications of its algorithms in a number of established areas of materials science and discusses the enhancements needed for applications in wild environments. This work committed to popularizing machine learning fundamentals and encouraging its application in materials science.

Wei, J., Chu, X., Sun, X.Y., Xu, K., Deng, H.X., Chen, J., Wei, Z. and Lei, M., 2019. Machine learning in materials science. *InfoMat*, *1*(3), pp.338-358

Accelerating Material Property Predictions using Machine Learning:

If we can successfully learn from the information and data that is already available, the materials discovery process can be greatly accelerated and simplified. In the current contribution, it has demonstrated how machine (or statistical) learning methods trained on quantum mechanical calculations combined with the concepts of chemical similarity can be used to efficiently and accurately predict a wide range of attributes of material systems.

Pilania, G., Wang, C., Jiang, X., Rajasekaran, S. and Ramprasad, R., 2013. Accelerating materials property predictions using machine learning. *Scientific reports*, *3*(1), p.2810.

Enhancing property prediction and process optimization in building materials through machine learning:
Large databases currently include a depth of knowledge on critical material properties as a result of a recent rise in experimental data availability. Utilizing this data along with Machine Learning (ML) tools can improve the effectiveness of the materials' manufacturing process.

Stergiou, K., Ntakolia, C., Varytis, P., Koumoulos, E., Karlsson, P. and Moustakidis, S., 2023. Enhancing property prediction and process optimization in building materials through machine learning: A review. *Computational Materials Science*, *220*, p.112031.

Machine learning-driven new material discovery:
This article reviews the research on applying machine learning to the discovery of new materials, including data preprocessing, feature engineering, machine learning algorithms, and cross-validation techniques. It then suggests using machine learning to supplement conventional DFT calculations in the process of finding new materials.

Cai, Jiazhen, Xuan Chu, Kun Xu, Hongbo Li and Jing Wei. “Machine learning-driven new material discovery.” Nanoscale Advances 2 (2020): 3115 - 3130.

Accelerating materials development for energy storage and conversion:
The need for energy has increased in significance on a global scale with the growth of contemporary society. Therefore, there is a pressing need to investigate novel materials for sustainable energy systems. A long experimental period and high cost make traditional approaches difficult to use in materials research. Machine learning (ML) is currently emerging as a new research paradigm to transform the discovery of novel materials.

Chen, An, Xu Zhang and Zhen Zhou. “Machine learning: Accelerating materials development for energy storage and conversion.” InfoMat (2020): n. pag.

Deep Learning the Chemistry of Materials From Only Elemental Composition:
ElemNet is a deep neural network model that has been designed and put into use. ElemNet automatically detects the physical and chemical interactions and similarities between various elements using artificial intelligence, allowing it to predict the properties of materials more accurately and quickly.

Jha, Dipendra, Logan T. Ward, Arindam Paul, Wei-keng Liao, Alok N. Choudhary, Christopher M. Wolverton and Ankit Agrawal. “ElemNet: Deep Learning the Chemistry of Materials From Only Elemental Composition.” Scientific Reports 8 (2018): n. pag.

Machine learning approaches for the prediction of materials properties:
Numerous research teams have suggested using deep learning to solve issues in the chemical and materials sciences.Ma et al. trained a model with a set of ab initio adsorption energies and electronic fingerprints of an idealized bimetallic surface (spatial extent of metal d-orbitals, atomic radius, ionization potential, electron affinity, and Pauling electronegativity) using an ANN that was implemented in the open-source PyBrain code. When used to simulate the electrochemical reduction of carbon dioxide on metal electrodes, this model was able to represent complicated nonlinear interactions between the adsorbate and substrate.

Chibani, S. and Coudert, F.X., 2020. Machine learning approaches for the prediction of materials properties. *Apl Materials*, *8*(8).

Machine Learning for Property Prediction and Optimization of Polymeric Nanocomposites:
In order to more accurately predict the thermal, electrical, mechanical, tribological, and other desired properties of polymer nanocomposites, other key descriptors, such as the trap state (effects of chemical structures, additives, polymer-nanofiller interface, etc.), morphologies (linear, cross-linked, free volume, etc.), and processing conditions, should be incorporated into fingerprints. For structure-property analysis and property prediction, more sophisticated neural network algorithms (such as transfer learning, CNN, etc.) and inverse design techniques could be used.

Champa-Bujaico, E., García-Díaz, P. and Díez-Pascual, A.M., 2022. Machine learning for property prediction and optimization of polymeric nanocomposites: a state-of-the-art. *International Journal of Molecular Sciences*, *23*(18), p.10712.

Machine learning-based accelerated property prediction of two-phase materials using microstructural descriptors and finite element analysis:
It is discovered that artificial neural networks, principal component analysis, and two-point correlation (TPC) functions can all successfully forecast the homogenized elastic characteristics. Despite the fact that the PCs for each set of microstructures are distinct, distinguishable patterns are found to represent the essential microstructural characteristics for microstructure-based property prediction. Based on microstructural pictures, our work paves the way for the creation of ML algorithms that can forecast the mechanical characteristics of intricate, multi-phase microstructural composites.

Ford, E., Maneparambil, K., Rajan, S. and Neithalath, N., 2021. Machine learning-based accelerated property prediction of two-phase materials using microstructural descriptors and finite element analysis. *Computational Materials Science*, *191*, p.110328.

Evidential Deep Learning for Guided Molecular Property Prediction and Discovery:
Evidential deep learning may be especially applicable to uncertainty-guided virtual screening of huge chemical libraries due to its effectiveness and usability. Prior to prioritizing candidates for experimental validation, virtual screening methods frequently entail extensive prediction of the characteristics and performance of compounds in sizable virtual libraries. Evidential deep learning might make it easier to use uncertainty-aware neural models for molecular property prediction, discovery, and design in a robust and reliable way.

Soleimany, A.P., Amini, A., Goldman, S., Rus, D., Bhatia, S.N. and Coley, C.W., 2021. Evidential deep learning for guided molecular property prediction and discovery. *ACS central science*, *7*(8), pp.1356-1367.

Improving Material Property Prediction by Leveraging the Large-Scale Computational Database and Deep Learning:
Although several material training databases and property prediction models have been put out, it is still difficult to predict properties with any degree of accuracy. In this article, we present a "Matgen + CrystalNet" approach package to enhance material property prediction. One can create a large-scale material genome database (Matgen) with 76k materials taken from an experimentally observed database and compute their properties using the Perdew-Burke-Ernzerhof (PBE) functional in density functional theory.

Chen, P., Chen, J., Yan, H., Mo, Q., Xu, Z., Liu, J., Zhang, W., Yang, Y. and Lu, Y., 2022. Improving Material Property Prediction by Leveraging the Large-Scale Computational Database and Deep Learning. *The Journal of Physical Chemistry C*, *126*(38), pp.16297-16305.