Chapter 14
Advancing Material Property Prediction With AI and Deep Learning Technologies

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ABSTRACT

Artificial intelligence and deep learning technologies are driving transformations in material science, particularly in predicting material property through machine learning applications. In this chapter, we are concerned about how materials property prediction can be revolutionized by advances in new state-of-the-art technologies enabling more accurate and efficient predictions in comparison to the traditional methods which incur time-consuming and cost-consuming expense. While both ML and deep learning offer powerful alternatives, they require large datasets and robust algorithms to accurately map complex interplay between the material structure and its properties. In this text you will read about employing deep learning architectures, such as CNNs and RNNs, in predicting properties such as mechanical strength, thermal conductivity and electronic behavior. The chapter discusses successful case studies and predicts future material science research and industry practices integrating AI-driven approaches.

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INTRODUCTION

Ontology-based ceramic material property prediction in pyinput is an example of early research studies that exhibit trends towards the integration of similarity measure methodologies, making difference between ceramic properties (at least theoretical level properties) and structure among various approaches to machine learning in material property prediction. Material properties have traditionally been predicted largely through empirical testing and theoretical models. These approaches entail either performing physical experiments to probe material properties or applying basic equations to compute properties from material compositions and processing conditions. Although these methods yield beneficial information, they are commonly limited by their time-consuming, expensive, and inability to provide accurate value of intricate material characteristics(Ghosh et al., 2019).

Machine learning and AI has gained tremendous focus in recent times in bringing the solution to the problem space by offering several methodologies as alternative options to replace traditional techniques with more efficient and often delivering better results. AI is the extent to which a computer is capable of acting which requires human intelligence — learning, reason, problem solving, etc. A popular branch of AI called deep learning makes use of artificial neural networks with multiple layers that can teach themselves to learn from massive amounts of data and identify complex correlations. Such capabilities make AI and deep learning especially well-suited for material property prediction, where the relationship between material structure and property is often complex and multi-dimensional(Wang & Adachi, 2019).

There are multiple motivations for AI integration into material science. The acceleration has been threefold: First, the rapid development in computational technologies has made it possible to analyze large amounts of data faster and with greater efficiency. The growth has been greatly spurred by the rise of large datasets from experimental measurements, computational simulations, and theoretical calculations. These data sets are used to train deep learning models, which can discover patterns and correlations that may not be possible through traditional methods. As an example, CNN can be used to capture and learn spatial characteristics of material micro-structures; on the other hand, RNN is particularly useful to deal with sequence data, e.g., so that it can be effective to predict time-dependent properties (Chen et al., 2020).

A significant benefit provided in leveraging AI for material property predictions lies in handling high-dimensional data. As an example, in material science this typically requires the integration of different types of data such as chemical formulas, preparation condition, experimental outcomes. This information can then be synthesized by a deep learning model to accurately predict material properties, recieving high performance when compared to traditional models that may fail at the same complexity. They were applied to predicting mechanical properties like tensile strength and hardness, thermal properties like conductivity and expansion, and electronic properties such as conductivity and band gap (Chibani & Coudert, 2020).

One of the main advantages of technologies like AI and deep learning is their ability to accelerate the discovery and optimization of new materials. Traditional approaches can be costly and time-consuming, relying on extensive trial-and-error experimentation. Researchers utilize the power of AI to predict the properties of the materials even before the physical tests are done which speeds up the entire development process. This ability is especially important in sectors such as aerospace, automotive, and electronics where it is essential for material performance and there exists a high demand for novel materials (Dai et al., 2020).