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Materials characterization: Can artificial intelligence be used to address reproducibility challenges?

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ABSTRACT

Material characterization techniques are widely used to characterize the physical and chemical properties of materials at the nanoscale and, thus, play central roles in material scientific discoveries. However, the large and complex datasets generated by these techniques often require significant human effort to interpret and extract meaningful physicochemical insights. Artificial intelligence (AI) techniques such as machine learning (ML) have the potential to improve the efficiency and accuracy of surface analysis by automating data analysis and interpretation. In this perspective paper, we review the current role of AI in surface analysis and discuss its future potential to accelerate discoveries in surface science, materials science, and interface science. We highlight several applications where AI has already been used to analyze surface analysis data, including the identification of crystal structures from XRD data, analysis of XPS spectra for surface composition, and the interpretation of TEM and SEM images for particle morphology and size. We also discuss the challenges and opportunities associated with the integration of AI into surface analysis workflows. These include the need for large and diverse datasets for training ML models, the importance of feature selection and representation, and the potential for ML to enable new insights and discoveries by identifying patterns and relationships in complex datasets. Most importantly, AI analyzed data must not just find the best mathematical description of the data, but it must find the most physical and chemically meaningful results. In addition, the need for reproducibility in scientific research has become increasingly important in recent years. The advancement of AI, including both conventional and the increasing popular deep learning, is showing promise in addressing those challenges by enabling the execution and verification of scientific progress. By training models on large experimental datasets and providing automated analysis and data interpretation, AI can help to ensure that scientific results are reproducible and reliable. Although integration of knowledge and AI models must be considered for the transparency and interpretability of models, the incorporation of AI into the data collection and processing workflow will significantly enhance the efficiency and accuracy of various surface analysis techniques and deepen our understanding at an accelerated pace.

I. INTRODUCTION

Following the remarkable success of artificial intelligence (AI) within the past few decades, there has been rapid advancement of AI being applied to different fields, such as in natural language processing,[1–4] robotics,[5,6] and many others. In materials science, we are just beginning to see the use of AI in the analysis of material characterization data from techniques such as x-ray photoelectron spectroscopy (XPS), extended x-ray absorption fine structure