

This critique is related on the content of Ch.01- Chemistry, Materials and, Nanoscience. Nowadays, thanks for the help of Artificial Intelligence (AI), wide range of science fields develop rapidly, including the topic the article talking about. Chemistry and materials science are the fundation of modern technology; in other word, developing methods to design and refine different material substances or chemical compounds can result in a huge improvement of modern technology. However, with the advancement of material science, the technology complexity is rised to a new level, which make it difficult to bring up or conduct experiments while looking for novel materials, and AI and Machine learning (ML) can offer a pathway to deal with the overwhelming complexity. In fact, AI and ML are already been used in the field, and the result is astonishing. For example, with the help of AI, the timeline of discovery of new batteries materials is reduce from 14 years to less than 5 years.

By analyzing multiple complex data and exploiting state-of-the-art ML can scientists accelerate discovery of new materials and chemical compound. To be precise, two major gaps between material design and discovery are shorten by the implement of AI. Firstly, the combination of growing High-performance-computing capabilities and efficient electronic structure calculation method allow scientists to explore various materials virtually. Nevertheless, the precision and reliability of the simulation required further enhancement. Secondly, through applying all the data contained in experiments and calculations, researcher can predict and understand unknown materials. One of the applications is a method, which is based on deep learning (DL), used to identify enumerate defects.

The goal of the application of AI regarding the field of chemistry and materials science is to build autonomous smart experiments and simulations, including synthesis and automated discovery, which combines every part of materials and chemistry discovery loop. However, numerous challenges need to be solved to achieve the accomplishment, including mastering hierarchical architectures and beyond equilibrium matter; understanding the critical roles of heterogeneity, interfaces and disorder; transformative improvement in models, math, algorithms, data, and computing; exploiting coherence in light and matter; conducting revolutionary advances in imaging capabilities across wide range of scales. A few developments are crucial to address the problems mentioned above. Including, integration of experimental instruments and advance edge computing, enabling in situ multimodal analysis and physics representation by AI/ML methods and big-fast data at the signal-noise edge, and last but not least, creating a cross-domain workforce.

Moreover, with the help of AI and ML automation of model-building and decision-

making in experimental loops, scientist also predict that several fields, such as acceleration simulation, advancement of mathematical algorithms, enhancement in big data and data curation, detection off rare events, and so forth, will be significant improved.

If the challenge mentioned above been solved five revolutionary advances will happen. Firstly, the diversity of materials properties may breakthrough the limits drawn by equilibrium thermodynamics or previous discovered design rules. Secondly, the realization of multifunctional and self- regenerating catalytic systems. Thirdly, the interfaces perform desired function by manipulation. Forth, rapid chemical and biological materials design and synthesis. Fifth, the discovery of unknown synthesizable materials and complex chemical species 1000 times faster than previous cases.

The article provided lots of evidence to support the viewpoints that Artificial Intelligence and Machine learning can enhance the efficiency of the development of chemistry and materials science to the next level, though there are some challenges needed to overcome. Once the vision of autonomous smart experiments and simulations can be accomplished, not only can the timeline of discovering new materials shrink severely, but the cost that spend on countless experiments can also be saved. However, a well-trained materials science researcher is essential to ensure the viability and success of the program. Therefore, the program is not fully automated. Hope in the near future, a completely automated system can be created.