Editorial

Materials research in artificial intelligence era

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Jinwu Kang
Tsinghua University, China

Correspondence: Jinwu Kang, School of Materials Science and Engineering, Key Laboratory for Advanced Materials Processing Technology, Tsinghua University, Beijing 100084, China, Email kangjw@tsinghua.edu.cn

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Recently ChatGPT is such a shocking tool that almost everyone deems it can bring a revolution to our society in every sectors. ChatGPT, a large language model (LLM) developed by Open AI, is a kind of artificial intelligence (AI) tool, shortened from chat generative pre-trained transformer. Following ChatGPT, several similar tools sprouts and more are expecting, such as Bard by Google, Bing Chat by Microsoft, ERNIE Bot by Baidu. This is a new milestone of artificial intelligence. It is powerful, can answer your questions, write reports, generating pictures and programming codes, etc. But, can we utilize it to do research in materials science and engineering? Maybe many people will be surprised by this kind of questions. However, we really hope to apply this powerful tool into our scientific research.

Liu et al.,[1] actually asked ChatGPT by typing "Can you generate a CIF file for $NaZr_2(PO_4)_3$?". Then he got the answer "Certainly, Here's the CIF file for $NaZr_2(PO_4)_3$". A CIF file was generated, and a figure of $NaZr_2(PO_4)_3$ atomic lattice structure appeared. He gave some basic suggestions and comments about the results to ChatGPT. Then it rewarded with updated atomic structure figure. Here CIF file is a file format to archive and distribute crystal structure information of materials. This is really an amazing example, demonstrating the great potential for its application in materials research. That means ChatGPT definitely owns some knowledge base of materials, and can provide users with basic knowledge of materials science. One of its big advantages is the accepting of natural language like conversation, which makes the common use of the system is easy, and possible for everyone.

Badini et al.,[2] applied ChatGPT for G code optimization for additive manufacturing. The G code is a programming language used in the field of 3D printing, including a set of commands that provide specific instructions to the 3D printer on how to print a particular object. ChatGPT was able to successfully optimize fifteen printing parameters while considering a multitude of variables such as the type of material, printer, slicer, and resolution of issues like warping, bed adhesion, and stringing. The not-optimized G code resulted into failure of printing, while, the optimized one led to sound printed specimen with the prevention of bed adhesion and warping defects.

Actually ChatGPT is not the all of AI. AI consists of a lot of models, such as DNN (deep neutron networks), RNN (recurrent neutron networks), CNN (convolutional neutron networks), GAN (generative adversarial networks), Diffusion model, etc. It evolves from generation to generation, coming to be more powerful, faster and bigger. Ma et al.,[3] used GAN to expand 47 images of poly-crystalline iron to 136, and performance of the model based on the generated data with 35 % of the real data reached the same level of performance as that based only on the real data.

Stach et al.,[4] proposed an idea of autonomous experimentation system for materials development by using AI to help for decision for next phase of experiment and data analysis without human intervention.

AI has the potential for real-time optimization during the manufacturing process due to its time-saving capability. For example, it was able to optimize computationally multiple parameters in just 1 h for the above mentioned application[2] or in seconds usually for small scale problems. Therefore, it will be of significance to integrate AI tools such as ChatGPT into an control software platform of equipment or devices to provide real-time suggestions and optimization for users.

AI method can be also adopted to mine existing databases to identify potential materials and processes.

The absence of completely known underlying physics and chemistry of complex material systems, materials processing and fabrication, and manufacturing enhances the irreplaceable position of AI. It can serve as an alternative method for computational material simulation methods (e.g., density functional theory (DFT), molecular dynamics (MD), etc.) and numerical simulation methods (e.g., finite difference method (FDM), finite element method (FEM), etc.). AI can assist the steps through the whole life cycle of material discovery (including characterization, property prediction, synthesis, and theory paradigm discovery).[5]

However, there is still a tons of work to do to turn AI into a useful tool for the research in materials science and engineering. Firstly, to feed the AI system with highly formatted, large scale, professional materials database, which is the foundation for the generation of new results. Secondly, the interface to accept, professional expression of academic contents beyond natural languages, such as equations, formulas, tables, charts, figures, motions, voice, etc. I am confident that with the model and database improvements a eruption of research achievements will appear in recent years.

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Conflicts of interest

There are no conflicts of interest.

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