Applying machine learning to the design of materials for lithium ion battery

Wei Wu[1] and Qiang Sun[1,2,*]

[1]Department of Materials Science and Engineering, College of Engineering, Peking University, Beijing 100871, China
[2]Center for Applied Physics and Technology, Peking University, Beijing 100871, China

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Lithium ion batteries (LIBs) are widely used in electrical vehicle, portable electronic products and energy storage devices. It is in urgent need to develop novel battery materials with higher energy density, preeminent rate performance and better safety performance. Traditional experimental methods for developing new materials are time-consuming, while for conventional simulation methods a huge gap remains between computations and practical materials. In this regard, machine learning becomes promising due to its flexibility in dealing with complex problems. Since machine learning is a data driven method, no physical or chemical models are needed in the process. The results will be reliable as long as the data are consistent with the practical situation. An encouraging example is AlphaGo [1] that has exhibited the charm of machine learning.

Machine learning provides effective ways of searching for the candidate program space through data training and optimizing the program algorithm. Data and algorithm are the two key factors which determine the accuracy of the machine learning. In fact, data is the basis of machine learning; it provides the knowledge for computers to learn, as well as the criteria of evaluating algorithms. Choosing proper learning algorithms is the other key, which can improve the efficiency and accuracy of the system.

For LIBs, most cathode materials are transition metal oxides and anode materials are carbon based materials. As for electrolyte, liquid electrolyte dominates the market while solid state batteries are still under development. When exploring the structure-property relationships in LIBs, many factors must be considered. For example, large amounts of data will be generated during high-throughput screening and since the relationships between structures and properties in LIBs don't have a one-to-one correlation, it's hard to find potential links between the simulation results. In such a case, machine learning can play an important role by using data classification and regression. Besides, reverse design of materials may be feasibly implemented in machine learning. Different from the conventional methods from structure to properties, reverse design of materials begins with targeting the property of the materials and tries to search for satisfactory structures and compositions. Machine learning has the ability to find out the property-to-structure relationships due to its flexibility in mapping complex relations.

It is very encouraging to notice that machine learning has already been put into predicting some properties of LIBs. For instance, Shandiz et al. applied different algorithms to classify silicate-based cathode [2]. Tanaka et al. used support vector machine algorithm to predict the ionic conductivity for superior lithium ion conducting solids [3]. Furthermore, a combination of DFT computations with machine learning methods was applied to the screening of garnet-type [4], olivine-type [5,6] and tavorite-type [7] materials. Besides, machine learning has also been used to study the cycling performance of LIBs. Since lithium ion battery is a dynamic system, the internal physical or chemical mechanisms are very complicated which makes it difficult to construct a simple model for estimating the remaining useful life. Different machine learning algorithms including relevance vector machine [8], particle filter [9], genetic algorithm [10] and support vector machine [11] have been used to estimate the remaining useful life and capacity degradation [12-15] of LIBs.

In short, machine learning is an emerging branch of artificial intelligence with great potential in developing novel lithium ion battery materials, and it deserves full attention from the researchers due to its flexibility in dealing with complex problems in practical conditions. However, some limitations exist for machine learning: Firstly, machine learning is a data driven approach, so the prediction is based absolutely on mathematical statistics, the physical or chemical significance need to be further studied; Secondly, a dataset with suitable size and accuracy is needed in machine learning, and it is of vital importance to choose proper data and do the pre-processing, while currently there only exist several commercial lithium ion battery systems, the available data are limited; Thirdly, optimum algorithms need to be improved for accuracy and efficiency. Since machine learning is still in the early stage, there is still a lot of work to be done in the future that include: (1) Reliable data selection and effective pre-processing; (2) Developing effective algorithms; (3) Integrating machine learning with other physics methods such as density functional theory and molecular dynamics for effective design of new battery materials.

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***Correspondence to:**

Qiang Sun
Department of Materials Science and Engineering
Peking University
China
E-mail: sunqiang@pku.edu.cn