LITHIUM-ION BATTERIES

Machine-learning design

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Computation can speed up the design of battery materials relative to purely experimental trial-and-error approaches, but the computational cost can be prohibitively high because high-accuracy and large-scale simulations are often required. Machine learning algorithms such as artificial neural networks (ANNs) can learn and make predictions based on input data so that computational efforts can be greatly reduced. However, applications of such algorithms in battery design are extremely rare. Now, Wei Lu and colleagues at the University of Michigan develop an efficient ANN methodology for the prediction of energy and power density, two important battery performance indicators.

In their approach, the researchers first identified six design variables as the inputs for the methodology. These included electrode thickness, porosity and applied C-rate (a measure of the rate at which a battery is (dis)charged with respect to its maximum capacity); a large dataset of variables (900 in total) was subsequently generated using design-of-experiments algorithms, which were then fed into a thermo-electrochemical finite element method (FEM) simulation. They then constructed ANNs from the input variables and the outputs of the FEM simulation. The machine-trained neural networks enabled them to perform 10,000 sets of Monte Carlo simulations, from which the energy and power density were generated. Furthermore, the ANN approach improves the simulation speed by several orders of magnitude compared to conventional methods while maintaining accuracy. The researchers discuss the effects of inputs on the performance indicators and single out the electrode thickness, porosity and C-rate as the key variables.

Changjun Zhang

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