A neural network based approach to predict high voltage li-ion battery cathode materials

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Abstract

This paper introduces the concept of using Artificial Neural Network (ANN) techniques for predicting electrochemical potential of cathode materials in combination with first-principles based quantum mechanical calculations. The proposed method can be used to predict the Lithium ion battery voltage if a new material is chosen as cathode. The methodology has low time-space complexity of computation and aims to integrate ANN with quantum mechanics based Density Functional Theory (DFT) calculations for accelerated insertion of new materials into engineering systems. It can be helpful in establishing new structure property correlations among large, heterogeneous and distributed data sets. ANN based modelling opens up the opportunity of screening large number of lithium based compositions for identifying promising materials within limited time and computational resources and can be further extended to all other battery materials.

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