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MACHINE LEARNING MODELS FOR PREDICTING THE DENSITY OF SODIUM-ION BATTERY MATERIALS

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Abstract

With unprecedented amounts of materials data generated from experiments, density functional theory and high-throughput density functional theory calculations, machine learning techniques provide the ability to accelerate the discovery and design of novel materials. In this paper, machine learning models that are capable of predicting the densities of sodium-ion battery (SIB) cathode materials were developed. Different machine learning models were developed and validated using SIB materials' properties calculated from DFT as input dataset, with the models' efficiency based on elemental properties of materials constituents as feature vectors. Machine learning models based on Bayesian ridge, gradient boosting regressor, light gradient boosting machine, extra trees regressor, random forest algorithms, and orthogonal matching pursuit were developed and evaluated. Extra trees regressor was found to be the best model in predicting the materials density with accuracy measures of 0.95 and 0.09 for coefficient of determination and mean square error, respectively. Also, the results show that maximum mass specific heat capacity and variance of DFT energy per atom descriptors are the most essential in accurately predicting the materials density.

Apply to be considered for a student ; award (Yes / No)?

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MSc

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