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MACHINE LEARNING MODEL FOR PREDICTING FORMATION ENERGIES FOR LITHIUM-ION BATTERY MATERIALS

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Abstract

Machine learning methods have recently found applications in many areas of physics, chemistry, biology and materials science, where large datasets are available. In this paper, machine learning methods are used to predict the formation energies of lithium-ion battery (LIB) materials. Thus, using LIB materials' properties calculated from density functional theory as an input dataset, as well as feature vectors from properties of chemical compounds and elemental properties of their constituents, different machine learning algorithms are explored in order to predict the formation energies for the battery materials. Models based on different algorithms, i.e., extremely randomized trees, gradient boosting, light gradient boosting machine, catboost and random forest were developed and evaluated. The catboost regressor model was found to be the best model in predicting the formation energies, with accuracy of 0.95 and 0.06 for coefficient of determination and mean square error, respectively. Thus, the features used to predict the formation energies have predictive capability with a high accuracy.

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

Yes

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Hons

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