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FERMI ENERGY PREDICTION OF SODIUM-ION BATTERY CATHODE MATERIALS: A MACHINE LEARNING REGRESSION APPROACH

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Abstract
Transitioning from fossil fuels to renewable energy sources is a critical global challenge, it demands advances at the materials, devices for the efficient storage and management of renewable energy. Energy researchers have begun to incorporate machine learning techniques to accelerate these advances. In this perspective, machine learning regression techniques are applied to a large amount of data to develop machine learning models that predict the Fermi energy of sodium-ion battery (SIB) cathode materials accurately. Thus, the importance of feature vectors were evaluated based on the properties of the chemical compounds and the elemental properties of materials constituents, with the estimated FCC lattice parameter, the average electronegativity, and the average density proving to be the most significant descriptors to predict Fermi energy. Based on the evaluation of various models, the light gradient boosting machine model was found to be the most accurate at predicting the fermi energy, with coefficient of determination and mean square error of 0.82 and 0.52 eV, respectively.

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

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

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