
Contribution ID: **174** Type: **Oral Presentation**

# DEVELOPMENT OF MACHINE LEARNING MODELS FOR PREDICTING ENERGIES OF SODIUM-ION BATTERY MATERIALS

*Monday, 4 July 2022 15:15 (15 minutes)*

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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 regression techniques are applied to a large amount of density functional theory calculated data to develop machine learning models capable of accurately predicting the formation and total energy of sodium-ion battery (SIB) cathode materials. Thus, Feature vectors importance derived from properties of materials' chemical compounds and elemental properties of their constituents was evaluated and found average covalent radius and average single bond covalent radius to be the most important descriptor for predicting the formation and total energy. Amongst various algorithms that were evaluated Bayesian ridge model was found to be the best model in predicting the formation energy and total energy, with accuracy of 0.99, 0.98 and 0.01, 0.03 for coefficient of determination and mean square error, respectively. The results show that the descriptors used to predict the energies have predictive capability with a high accuracy

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

Yes

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

MSc

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**Session Classification:** Physics of Condensed Matter and Materials

**Track Classification:** Track A - Physics of Condensed Matter and Materials