

Exploring cathode materials for batteries through machine learning

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Machine learning (ML) in materials science is becoming nowadays widely used for the estimation of material properties with precision comparable with previous techniques, typically based on density functional theory (DFT). The advantages of ML over DFT-based methods are its increased speed and the reduced computational costs. This can help materials scientists to screen enormous quantities of materials to find the best choices for their application of interest and accelerate the process of discovering new materials. In particular, advanced ML methods can be employed for analyzing different cathode materials to find viable alternatives to the widely used lithium-ion batteries, hopefully more efficient, safe and environmentally friendly. In our work, we adopt the graph neural network called GeoCGNN (namely geometric-information-enhanced crystal graph neural network) to predict formation energy per atom and redox potential of cathode materials. These are two important ingredients for meeting efficiency and safety requirements in batteries. This neural network has already shown in the literature to be more accurate in predicting various properties of crystals compared to other crystal graph neural networks and it is therefore extremely well suited for our task. We then apply it to screen many different Na-based cathode materials with varying amount of Ti, Ni and Ti to find the best choice for battery applications.