全機械学習によるハイスループット第一原理計算の代替の可能性

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Possibility of replacing high-throughput first-principles calculation by machine learning
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　　In recent years, due to the development of deep learning, the environment of material search using computers is about to change. In the normal material search flow, there are parts that require a relatively high calculation load, so-called calculation time. An example of this is the part that optimizes the structure by relaxation calculation when the structure of the material is input. At that time, first-principles calculations were used, but since continuous calculations have been developed and high-throughput calculations have been made, it has become possible to calculate all existing structures. In the background, with the discovery of the crystal graph neural network in 2018, a new trend was born to learn the results accumulated by high-throughput computation. One example is machine learning potential. It has been found that the results of first-principles calculations, which used to take a long time, can be predicted instantaneously. We aim to commercialize an all-solid-state lithium-ion battery for the purpose of making it practical. The purpose was to search for promising materials with high ion transport ability from among a huge number of candidate materials. We verified whether it can be an alternative to the first-principles calculation.
KEY WORDS: **EV and HV systems, All solid-state Li ion battery, Materials exploration, Materials simulation, Crystal Graph Neural Network, Machine Learning potential**

　　近年,深層学習の発展により，計算機を用いた材料探索の環境が変わろうとしている．通常の材料探索のフローには，比較的計算負荷の高い，いわゆる計算時間がかかる部分が存在する．その一例が，材料の構造を入力したときの緩和計算による構造の最適化の部分である．その時，用いるのが第一原理計算になるが，この計算も連続計算が発展し，ハイスループット化がされてきたため，既存の構造については，すべて計算してしまうということが可能になった．そういう背景の中, 2018 年の結晶グラフニューラルネットワークの発見に伴い，ハイスループット計算で蓄積した結果を学習させるという新たな潮流が生まれた．その一例が，機械学習ポテンシャルになる．この機械学習ポテンシャル [1,2]を用いることにより，従来の時間がかかっていた第一原理計算の結果を瞬時に予測できることがわかってきた．今回, 我々はハイブリッド(HEV),電気自動車(EV)の航続距離向上と安全化，長寿命化のために，全固体型リチウムイオン電池の実用化を目指しており．非常に膨大な材料候補の中からイオン輸送能の高い有望な材料を探索 [3,4]しなければならない．この目的のために，機械学習ポテンシャルが第一原理計算の代替となるのかを検証した．

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