Toward Discovery for Novel Solid Electrolytes for Li Ion Battery

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Lithium-ion rechargeable batteries are recognized as most promising power sources for electric vehicles, but they are limited by technical problems related to safety concerns linked to the use of flammable organic liquid electrolytes. Therefore, development of solid electrolytes using nonflammable oxides for an allsolid-state battery design is urgently requested. So far, several oxides such as β-alumina, LISICON, NASICON, perovskites, garnets, and so on, have been intensively studied as they demonstrate relatively good base Li ion conductivity. On the other hand, efforts are growing as well towards expanding the choice of candidate materials via discovery of new compositions or compounds from reported crystal structures, this is in the hope of speeding up the needed technical breakthrough..

Conventional materials search is often carried out through experimental trial-and-error approach based on researchers' knowledge/experience/intuition. Instead, we apply "data science" driven approach combined with state-of-art materials simulation techniques for search of novel solid electrolytes. In detail, we focused on the olivine and tavorite-type structures (Figure 1), since they are known as positive electrode compounds showing electrochemical stability and high-rate performance. Using density functional theory (DFT) and artificial neural network (NN) regression techniques, we successfully demonstrated the efficient and reliable conductivity prediction (Figure 2). In addition, extension of above mentioned techniques, we also succeeded to predict efficiently for next-gen. sodium ion batteries with the inclusion of thousands of inorganic compounds with various structures.

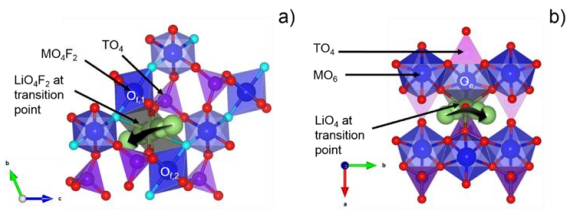

Fig. 1 Crystal structures of a) Tavorite and b) Olivine

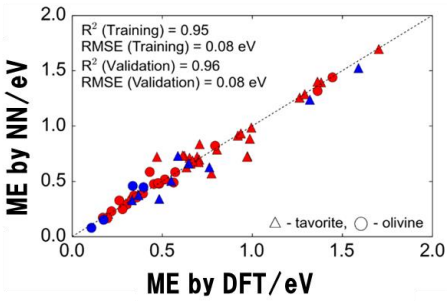

Fig.2 Diagnostic plots of conductivity property obtained by DFT and NN methods.

Bibliography

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