

Comprehensive exploring for cathode materials of fluoride ion batteries

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Fluoride-ion batteries (FIBs) are expected to replace lithium-ion batteries due to their high theoretical capacity. In order to utilize multinary alloys as cathode materials for FIBs, we've been exploring novel materials using "materials informatics," in which numerous alloy thin films are fabricated and their properties are predicted by machine learning based on evaluation and analysis data. Especially, for the XRD data, we focused on the dimension reduction using non-negative matrix factorization (NMF) to extract useful features. However, the conventional NMF is not suitable because it decomposes the peak-shifted XRD spectra into different features (basis vectors). But recently, "NMFk" has been reported, in which peak-shifted spectra are clustered into the same features, so we applied it to the data of Bi-La-Cu alloy thin films. The result of decomposing 181 spectra into 5 basis vectors, unlike conventional NMF, showed all of them were unique. Furthermore, compared to known structures, the major basis vectors were found to represent hcp and fcc structures. It indicates they are highly interpretable. In this presentation, we will report the results of regression learning using the above features as explanatory variables and cyclic voltammetry data as objective variables, and maximization of the objective variables using Bayesian optimization.