Materials design of electrolytes based on the DFT-MD simulation and informatics science.

Keiatro Sodeyama（NIMS, MaDIS, Group Learder）

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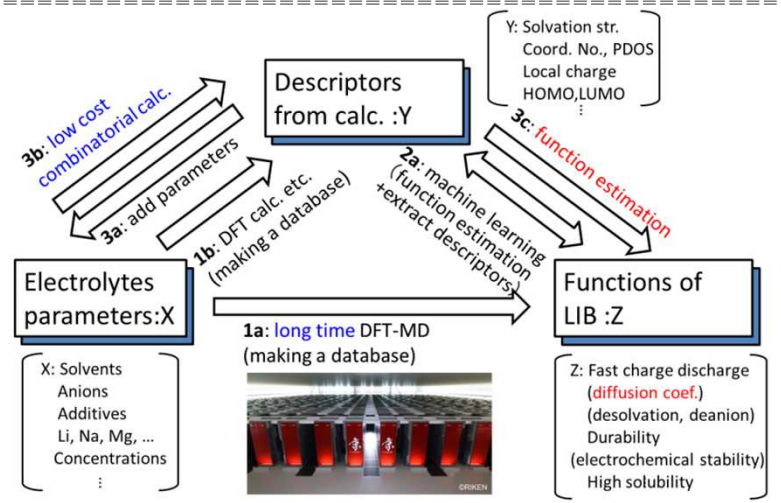
Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences（PO：Shinji Tsuneyuki）

Brief overview

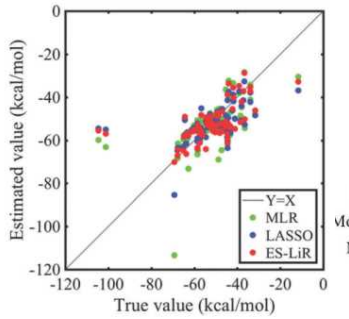
Exploring new liquid electrolyte materials is a fundamental target for developing new high-performance lithium-ion batteries(LIB). In contrast to solid materials, disordered liquid solution properties have been less studied by data-driven information techniques. To predict novel LIB liquid electrolytes with desired properties by the information techniques, we constructed a database of known liquid electrolytes by first-principles calculations. Next, we extracted the best descriptors combinations for predicting the target properties with data-driven information techniques. From the results, we proposed the virtual screening scheme of materials search to discover new liquid electrolytes with desirable properties.

Achievement

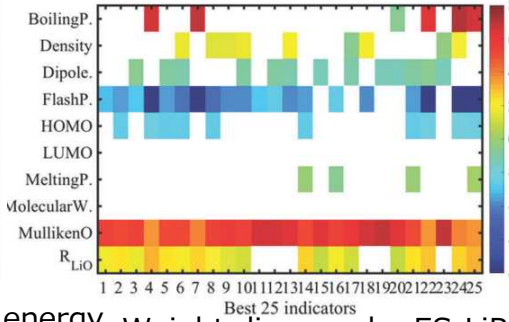
At first, we constructed a database of solvents (103 molecules from catalog) by first-principles calculations. Next, we extracted the best descriptors combinations with data-science techniques. We examined the estimation accuracy of multiple linear regression (MLR), LASSO, and exhaustive search with linear regression (ES-LiR), by using coordination energy as test liquid properties. We then confirmed that the ES-LiR gives the most accurate estimation among the techniques. We also found that the ES-LiR can provide the relationship between the “prediction accuracy” and “calculation cost” of the properties via weight diagram of descriptors. This technique makes possible to choose the balance of the “accuracy” and “cost” when the huge amount of new materials search carried out.



Liquid electrolyte informatics



Prediction of solvation energy



Weight diagram by ES-LiR

Reference/Link

1. “Liquid electrolyte informatics by exhaustive search with linear regression”, Keitaro Sodeyama, Yasuhiko Igarashi, Tomofumi Nakayama, Yoshitaka Tateyama, Masato Okada, *Phys. Chem. Chem. Phys.*, **20**, 22585–22591 (2018).

As for related strategic objectives related to this research area, see http://www.senryaku.jst.go.jp/teian/en/koubo/h29youkou_7_en.pdf