**Supporting Information**

**Chemical Composition-Driven Machine Learning Models for Predicting Ionic Conductivity in Lithium-Containing Oxides**†

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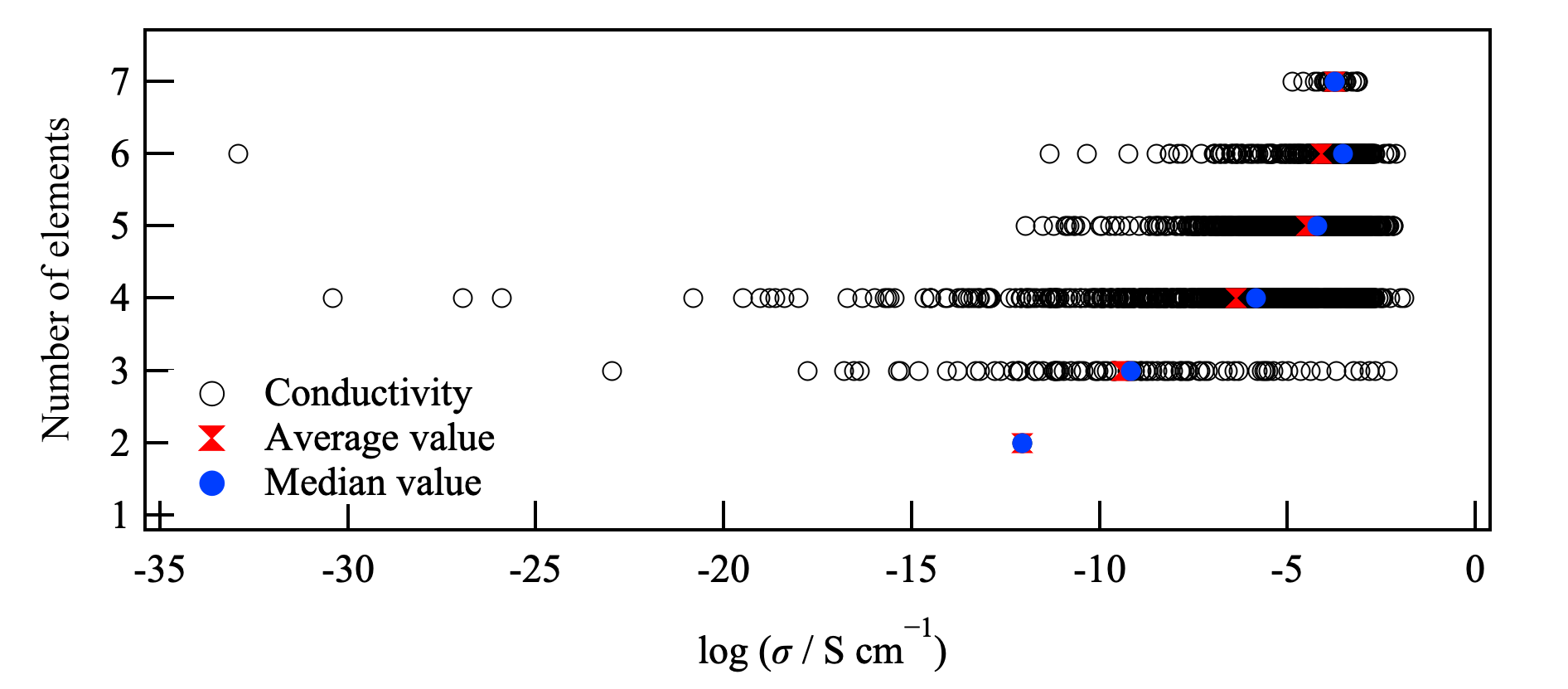


Fig. S1 Distribution of the material data for the number of elements and conductivity used for machine learning in this study. The average and median values of ion conductivity for each number of constituent elements are also represented.

ダイアグラム

AI によって生成されたコンテンツは間違っている可能性があります。

Fig. S2 Ionic-conductivity predictions for (1−*x*)Li2Si9O19–*x*Li2Mo9O28 using models that were not trained on lithium-free metal oxides data.

Table S1. Top 15 features with the greatest importance for the NGBoost and LightGBM models that were not trained on lithium-free metal oxides data.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| NGBoost | |  | LightGBM | |
| Feature | Importance (%) |  | Feature | Importance  (%) |
| Variance of "Vspd" (c,l) | 6.0 |  | "entropy" (c,l) | 14.7 |
| "entropy" (c,l) | 5.2 |  | Variance of "Vspd" (c,l) | 3.5 |
| Mean of "d" (c) | 4.1 |  | Content ratio of O | 3.5 |
| Mean squared of "d" (c) | 3.9 |  | Variance of "mp" (c,l) | 3.1 |
| Variance of "mp" (c,l) | 1.9 |  | Mean squared of "iV" | 2.9 |
| Content ratio of Si | 1.7 |  | Variance of "metal" (l) | 2.1 |
| Variance of "rp" (c) | 1.6 |  | Mean squared of "cs" (l) | 1.7 |
| Geometric mean of "val" (c,l) | 1.5 |  | Variance of "cV" | 1.7 |
| Mean squared of "iV" | 1.3 |  | Content ratio of Si | 1.4 |
| Content ratio of O | 1.3 |  | Mean squared of "d" (c) | 1.4 |
| "entropy" (l) | 1.3 |  | Mean of "d" | 1.3 |
| Content ratio of Sn | 1.3 |  | Variance of "s" (c) | 1.3 |
| Content ratio of Co | 1.3 |  | Mean of "d" (c) | 1.3 |
| Content ratio of Mo | 1.3 |  | Variance of "iV" (c,l) | 1.3 |
| Variance of "memnum" (l) | 1.2 |  | Variance of "memnum" (l) | 1.2 |