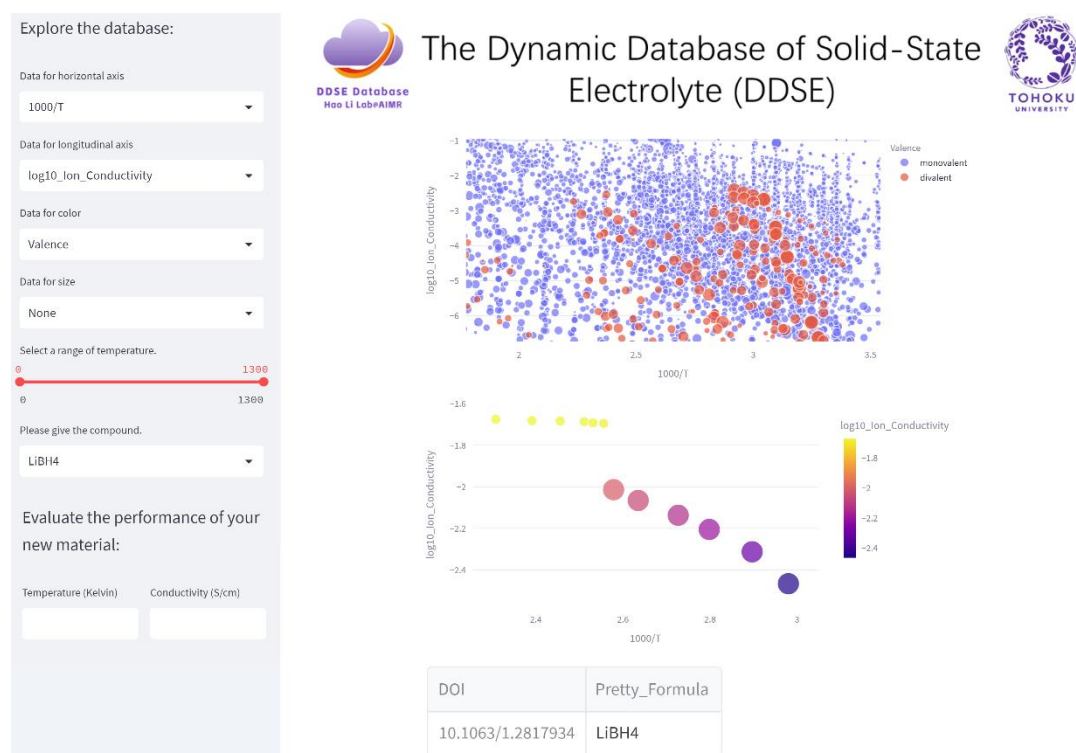


# User Instructions

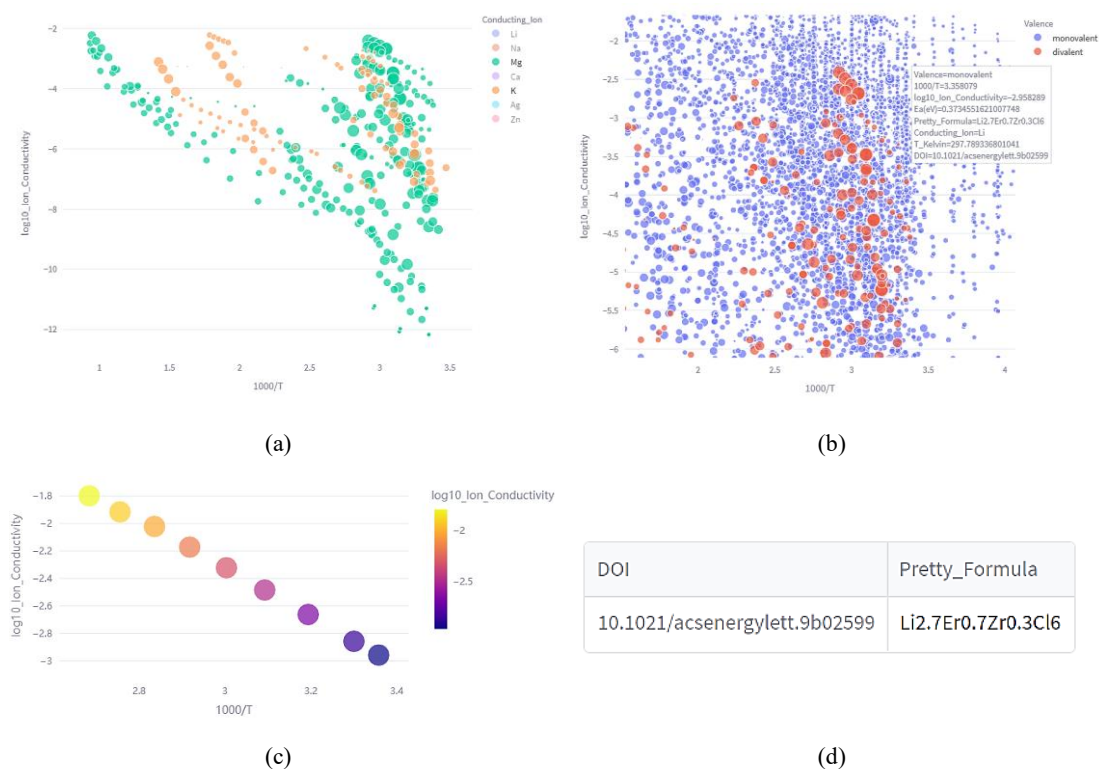
## 1. Information included in the DDSE

All materials in the dynamic database are collected from experimental values and contain abundant information, like activation energy, ionic conductivity, phase transform, and article source. Users can picture complex relationships between different materials' properties on this interface.



**Figure 1.** Interface of the DDSE.

The interface of our database is shown in **Figure 1** when you open this link (<https://ssbed-ssbed-database-gui-ntj1tz.streamlit.app/>). Users choose diverse materials' properties by the panel on the left side, and their relationships will be instantly shown in the exhibition region, which can be changed by selecting parameters from the top two lines. Meanwhile, other variates can be mapped to the plot in different colors and sizes to show more abundant information. For example, the different colors indicate the distribution of mono- and divalent materials in **Figure 1**, which can be severally shown by choosing one or the other in the legend. As the same method, the interface can show diverse conducting cations with different colors and can check each ion in the legend ( $\text{Mg}^{2+}$  and  $\text{K}^{+}$  shown in **Figure 2a**).



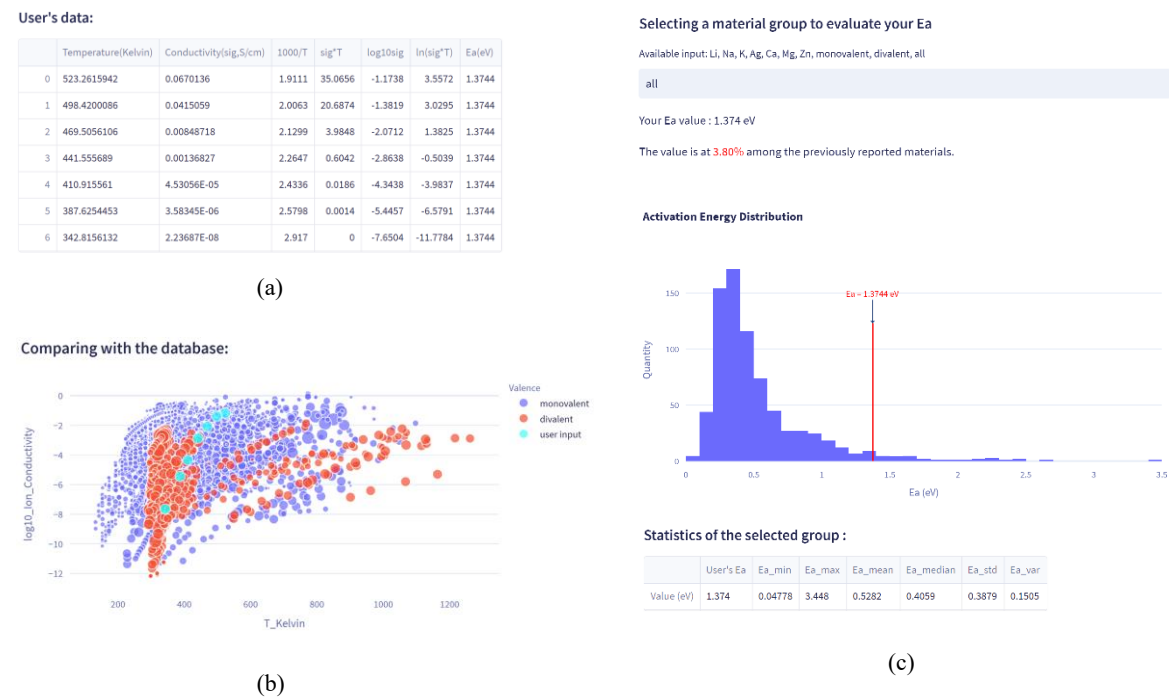
**Figure 2.** Distribution of the materials upon different screening methods. The diverse size of points indicates the activation energy  $E_a$ . (a) The distribution of  $\text{Mg}^{2+}$  and  $\text{K}^{+}$ , (b) distribution of the materials in the selected range, (c) properties of compound  $\text{Li}_{2.7}\text{Er}_{0.7}\text{Zr}_{0.3}\text{Cl}_6$ , (d) the literature source of  $\text{Li}_{2.7}\text{Er}_{0.7}\text{Zr}_{0.3}\text{Cl}_6$ .

Other regulations to screen materials are also supported, showing a specified temperature range by the free slider and selecting the data range they are interested in by zooming in the exhibition zone. And detailed information on a point can be obtained by selecting the one. **Figure 2b** demonstrates the distribution in selected regions and detailed information (in textbox) of compound  $\text{Li}_{2.7}\text{Er}_{0.7}\text{Zr}_{0.3}\text{Cl}_6$ . Meanwhile, the materials' ionic conductivity (**Figure 2c**) and source (**Figure 2d**) can be obtained when inputting the corresponding chemical formula at the last line of the panel. It is worth noting that the database is dynamic. We will add incessantly new materials, and the bottom of the interface records the total of materials and update time.

## 2. How to compare your new SSE's performance with previous literature reported to date?

Another important function is to compare and analyze the user's new material with all the collected compounds in the database. A demonstration was shown in **Figure 3**. The activation energy ( $E_a$ ) can be determined based on the Arrhenius equation when the user enters the temperature and corresponding ion conductivity in the panel (**Figure 1**). The user can adjust the characteristics of the coordinate axis through control panels to compare the distribution

of their data with the database. As shown in **Figure 3c**, the user can select a material group from the database to compare their data. The percentage and plot indicate the relationship between the user’s  $E_a$  and previously reported materials. The percentage is based on the formula  $(N/N_{\text{total}} \times 100\%)$ ,  $N$  represents the quantity in the database more than the user's  $E_a$  value, and  $N_{\text{total}}$  is the amount of all materials in the database). The data frame at the end of line evaluates the statistics of the selected group, including minimum ( $E_{a\_min}$ ), maximum ( $E_{a\_max}$ ), average value ( $E_{a\_mean}$ ), median ( $E_{a\_median}$ ), standard deviation ( $E_{a\_std}$ ), variance ( $E_{a\_var}$ ).



**Figure 3** A demonstration for comparison between the data of the user and database, (a) the related properties based on the user’s input, (b) the distribution of the input data in the database, (c) features of activation energy.

More novel and meaningful information can be obtained by exploring the difference in ionic conductivity between diverse materials, which can help us to understand the relationship between materials’ structure and performance. It can support for machine learning to predict and screen high-performance solid-state electrolytes.

### 3. More questions or feedbacks?

For more question or feedbacks, please contact Prof. Hao Li via: [li.hao.b8@tohoku.ac.jp](mailto:li.hao.b8@tohoku.ac.jp)