

Supplementary Information

Understanding the effect of oxide components on proton mobility in phosphate glasses using a statistical analysis approach

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S1. Linear Regression models

We first employed a general linear combination model, in which mol% of respective oxides are used as predictors, for both $\log(\mu_{\text{H}} \text{ at } T_{\text{g}})$ and T_{g} . The regression algorithm used in this study is based on the linear regression as implemented in MATLAB (MathWorks, USA). The obtained model for $\log(\mu_{\text{H}} \text{ at } T_{\text{g}})$ is as following:

$$\begin{aligned} \log(\mu_{\text{H}} \text{ at } T_{\text{g}}) = & -0.236388563x(\text{HO}_{1/2}) - 0.21732199x(\text{NaO}_{1/2}) - 0.128502192x(\text{WO}_3) \\ & + 0.671171102x(\text{NbO}_{5/2}) + 1.029198044x(\text{TaO}_{5/2}) + 1.374093231x(\text{MgO}) \\ & + 1.306366399x(\text{BaO}) + 1.971135165x(\text{LaO}_{3/2}) - 0.201698121x(\text{AlO}_{3/2}) \\ & - 0.284685842x(\text{YO}_{3/2}) + 1.859907493x(\text{GdO}_{3/2}) + 0.754725434x(\text{GeO}_2) \\ & - 0.629475199x(\text{BO}_{3/2}) - 0.293206847x(\text{PO}_{5/2}) \end{aligned} \quad (\text{S1})$$

Figure S1 shows comparison of experimentally observed and predicted values of $\mu_{\text{H}} \text{ at } T_{\text{g}}$. The root mean square error (RMSE) was 0.2278 and reasonably small. However, as shown in Fig. S2, the predicted values of $\log(\mu_{\text{H}} \text{ at } T_{\text{g}})$ for the 55,296 phosphate glass compositions (see the main text) were unreasonable in the range of $10^{-29} \sim 10^{17} \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$, although the range of the experimentally observed values is $2 \times 10^{-9} \sim 2 \times 10^{-7} \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$. This indicates that the overtraining occurred maybe because of small number of training data.

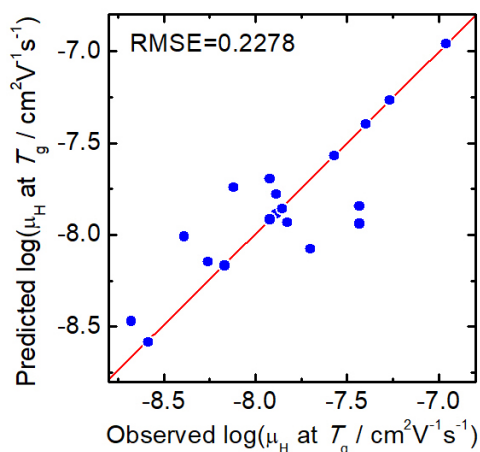


Figure S1. Comparison of experimentally observed and predicted values of $\mu_{\text{H}} \text{ at } T_{\text{g}}$

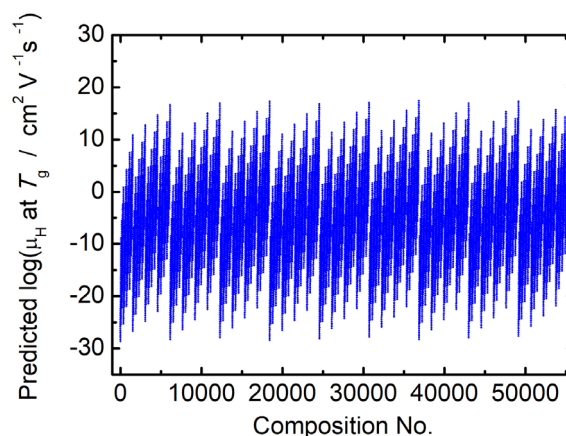


Figure S2. Predicted values of $\log(\mu_{\text{H}} \text{ at } T_{\text{g}})$ for the 55,296 phosphate glass compositions.