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Supplementary Information

Extracting higher-conductivity designs for solid polymer electrolytes by quantum-inspired annealing

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Table S1 Hyperparameter optimization of regression models.

Model	Hyperparameter	MAE
Ridge	$\alpha = 0.1$	2.31
Ridge	$\alpha = 1$	1.87
Ridge	$\alpha = 10$	1.51
Ridge	$\alpha = 100$	1.31
Ridge	$\alpha = 1000$	1.31
Quadratic	$\alpha = 0.1$	2.25
Quadratic	$\alpha = 1$	1.56
Quadratic	$\alpha = 10$	1.16
Quadratic	$\alpha = 100$	1.11
Quadratic	$\alpha = 1000$	1.16
Random forest	max_depth = 3	1.23
Random forest	max_depth = 5	1.21
Random forest	max_depth = 10	1.15
Random forest	max_depth = ∞	1.17

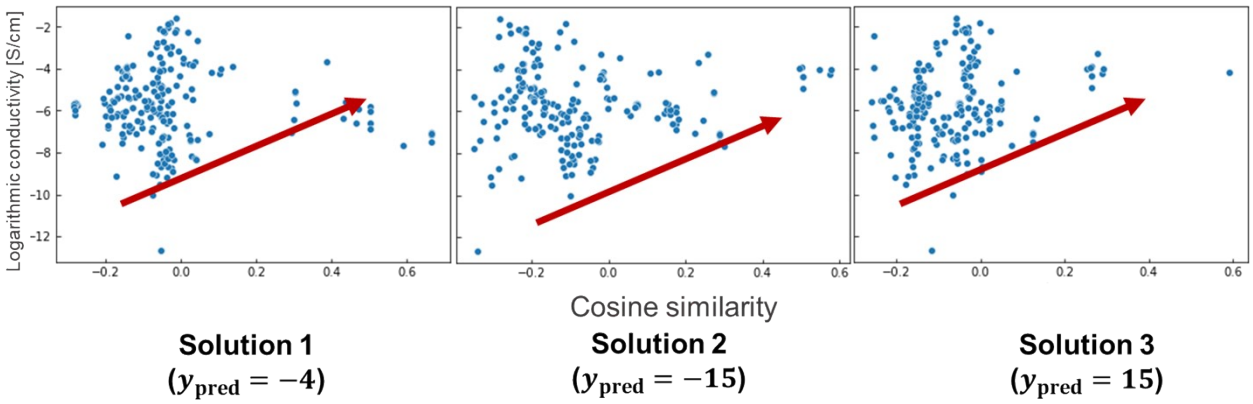
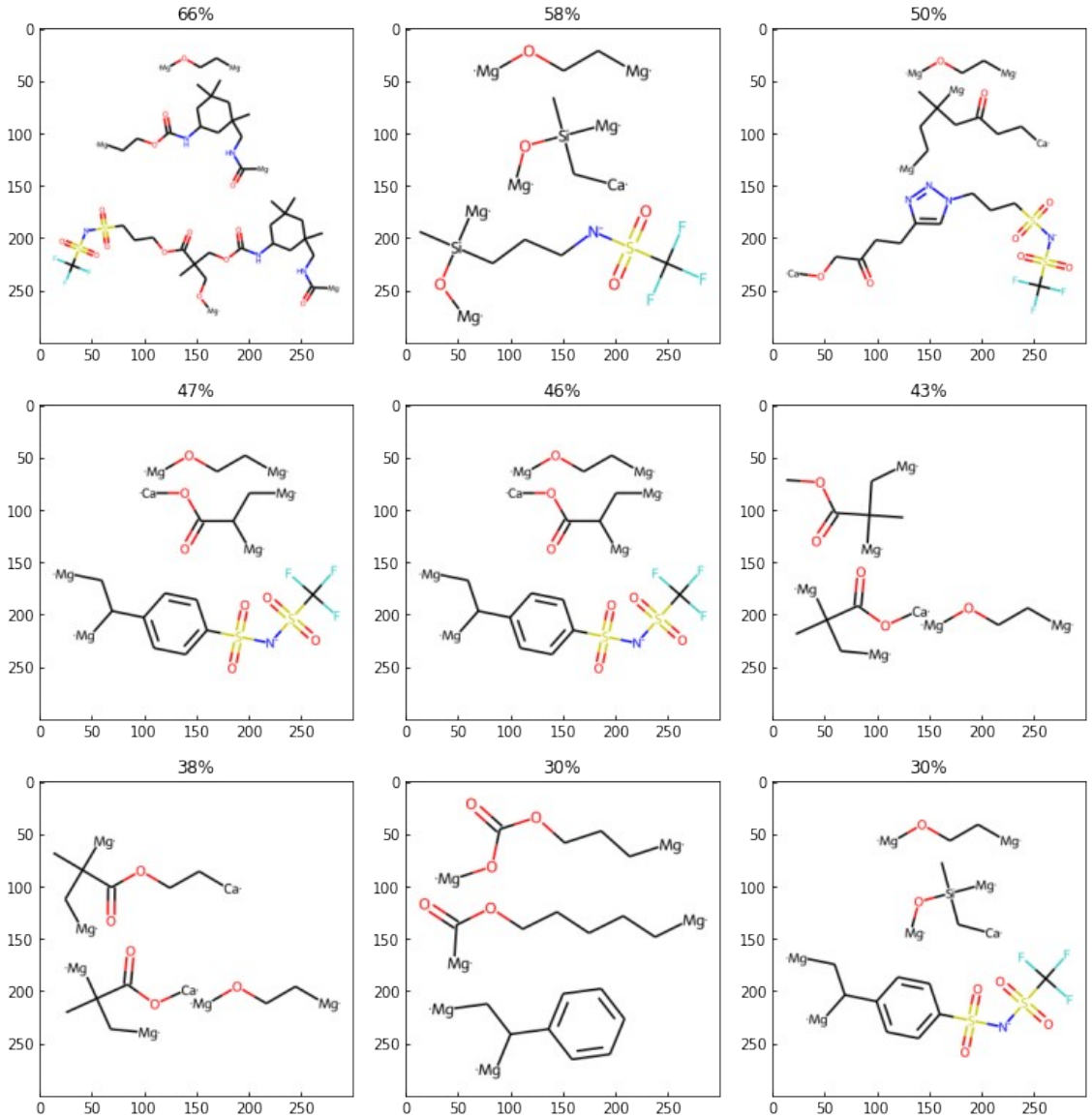


Fig. S1 Relationships between cosine similarity to ideal solutions X_{ideal} and experimental conductivities for the training dataset.



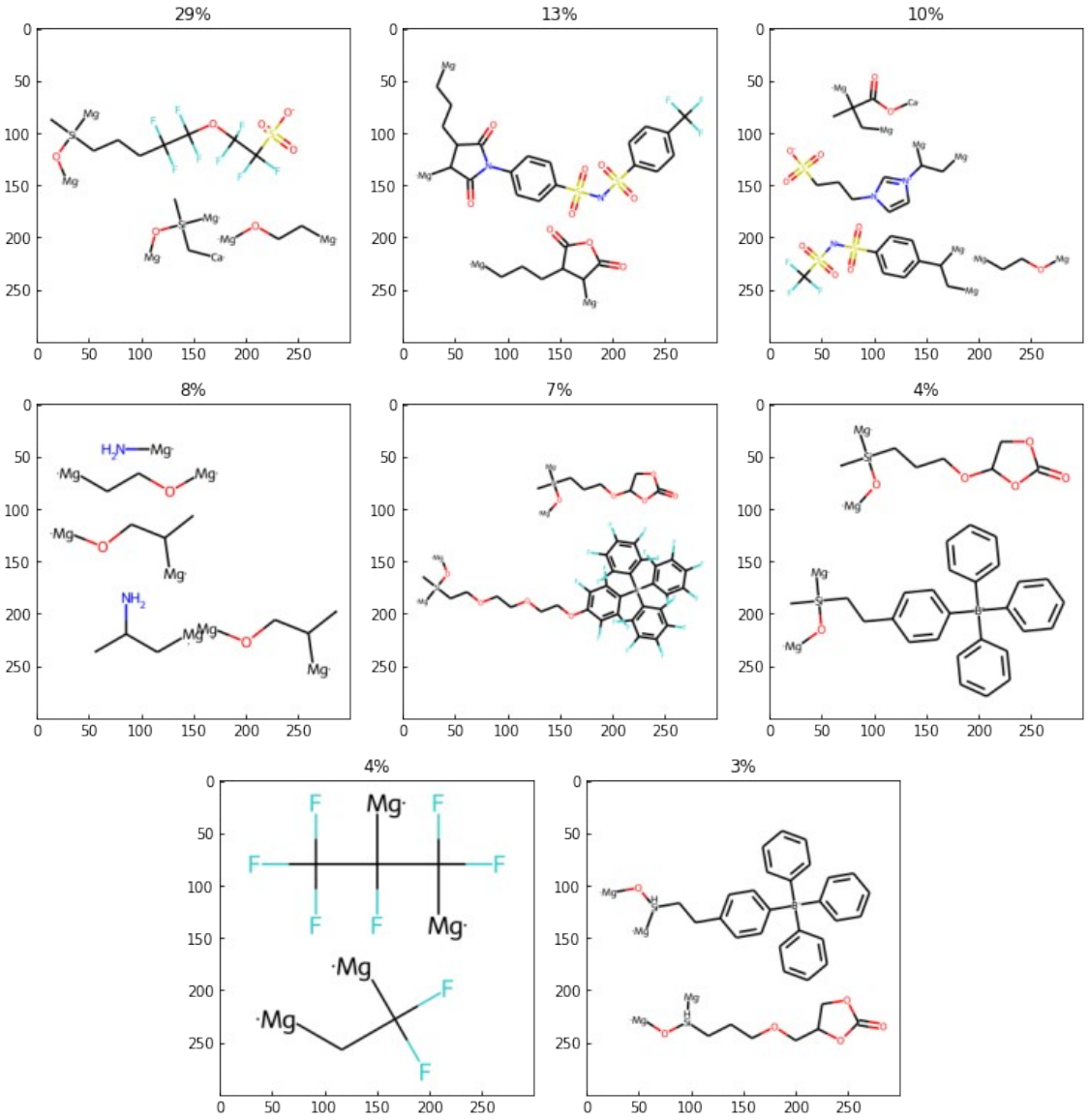
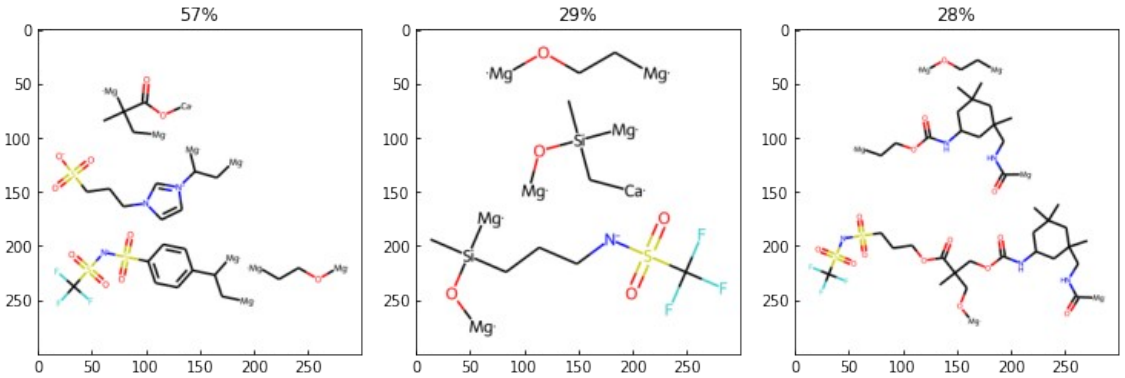


Fig. S2 Electrolyte structures similar to sampled solution 1. Cosine similarities are shown above the structure images. Repeating unit symbols are expressed as Mg or Ca atoms.



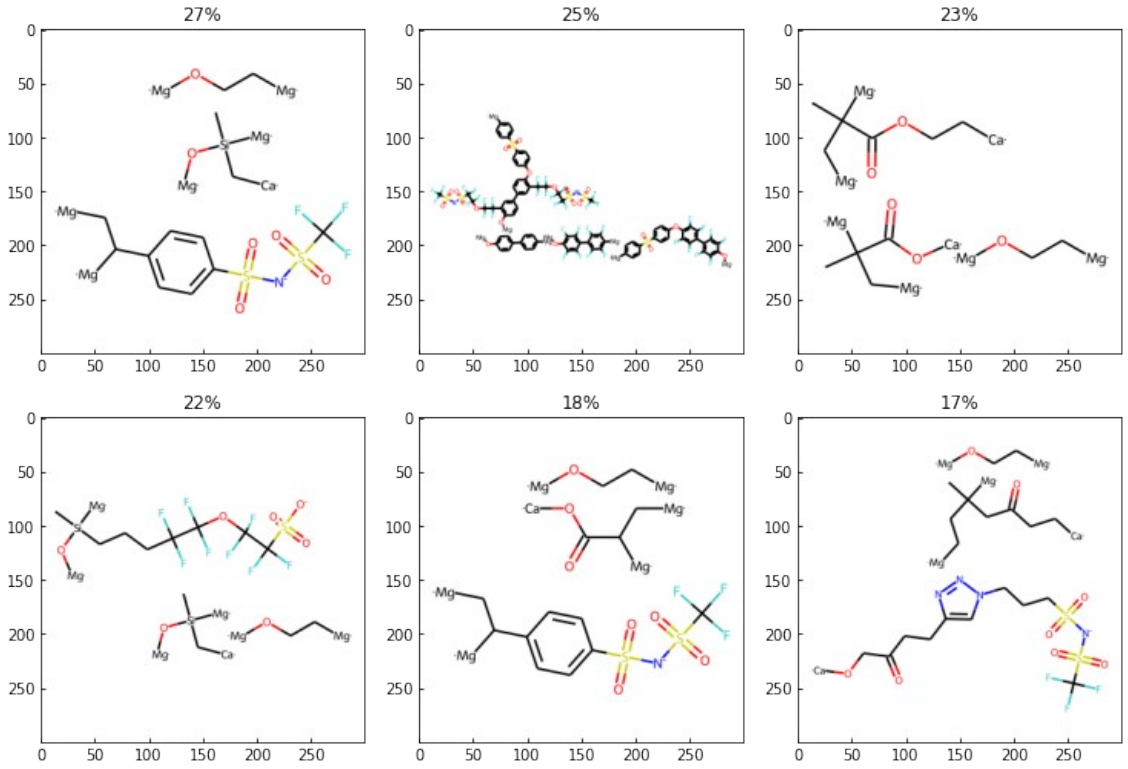
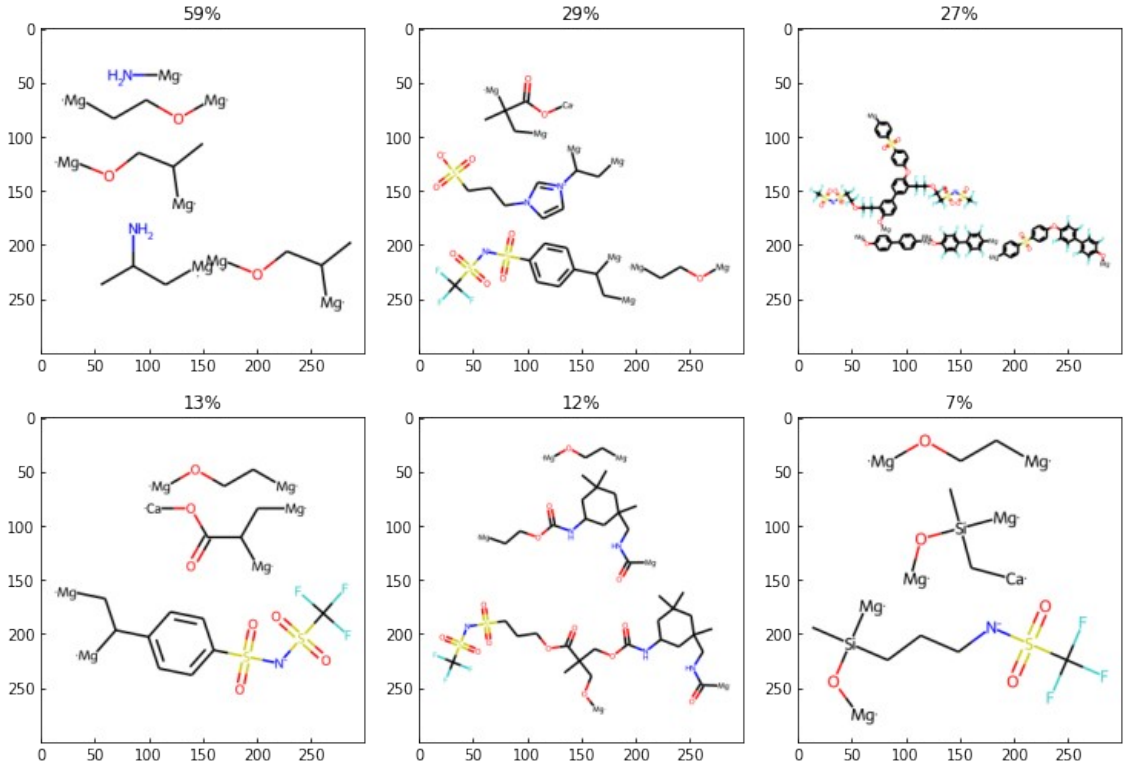


Fig. S3 Electrolyte structures similar to sampled solution 2. Cosine similarities are shown above the structure images. Repeating unit symbols are expressed as Mg or Ca atoms.



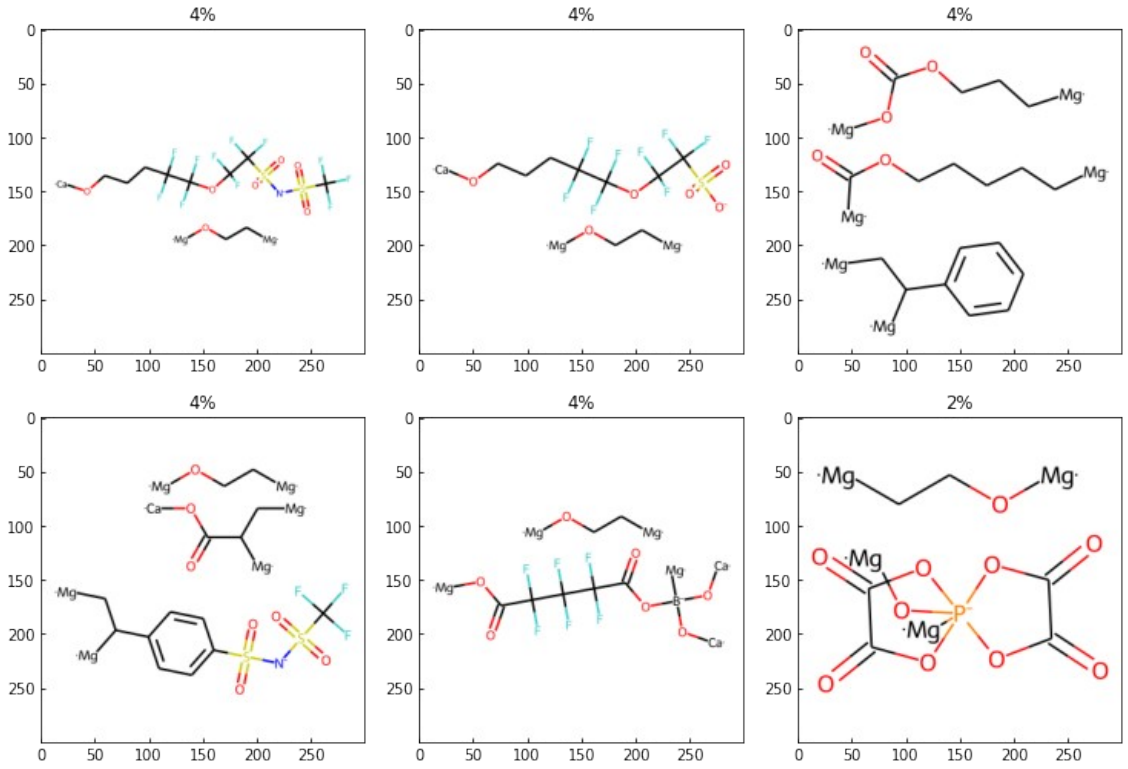


Fig. S4 Electrolyte structures similar to sampled solution 3. Cosine similarities are shown above the structure images.

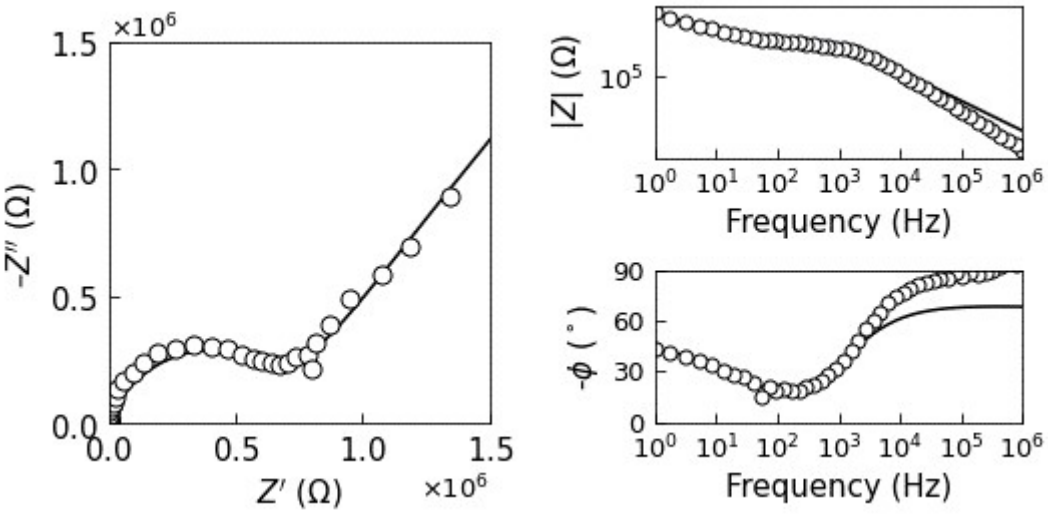


Fig. S5 Nyquist and Bode plots for the 5 mol % polymer composite.

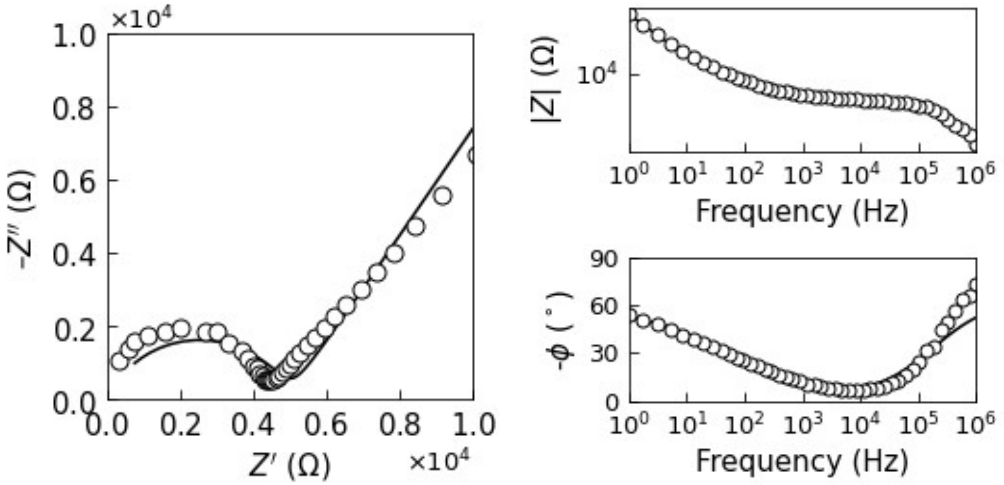


Fig. S6 Nyquist and Bode plots for the 11 mol % polymer composite.

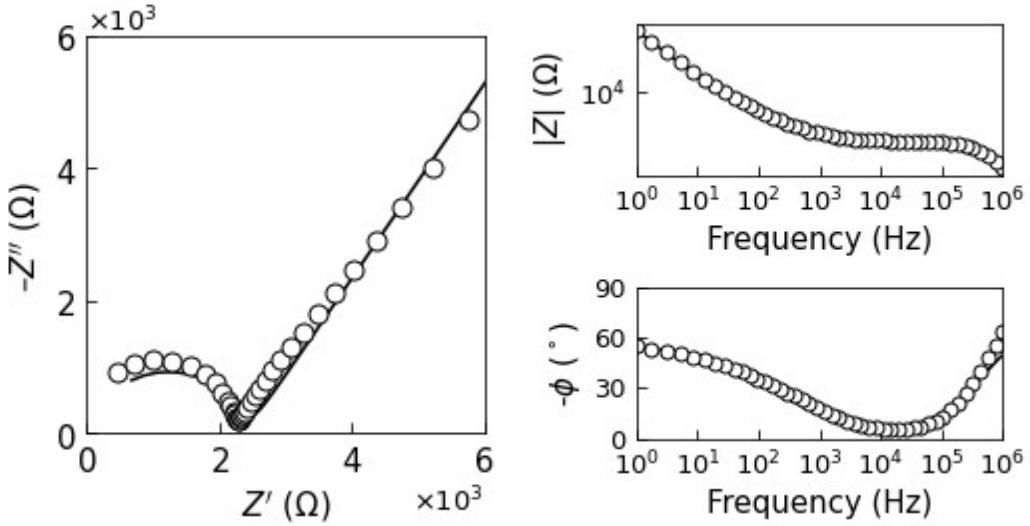


Fig. S7 Nyquist and Bode plots for the 25 mol % polymer composite.

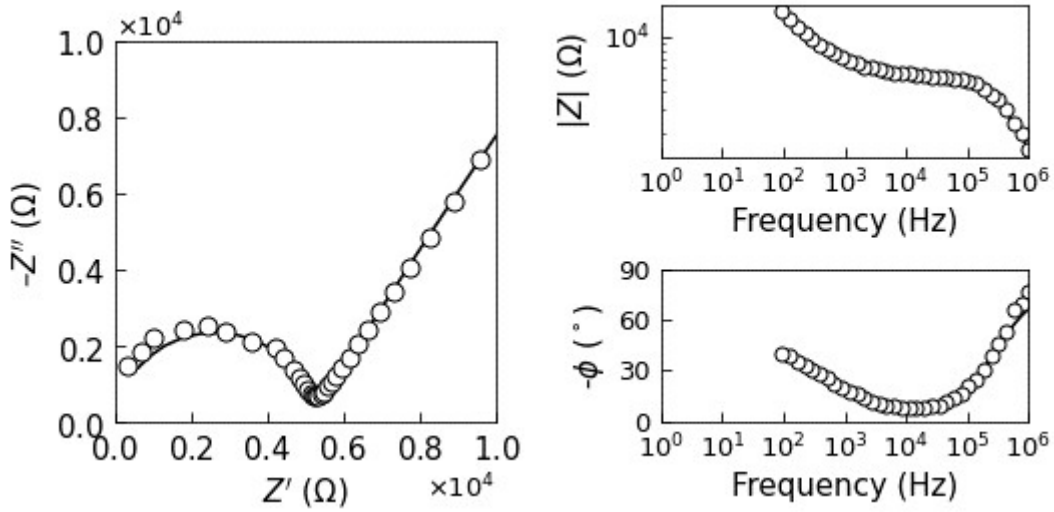


Fig. S8 Nyquist and Bode plots for the 33 mol % polymer composite.

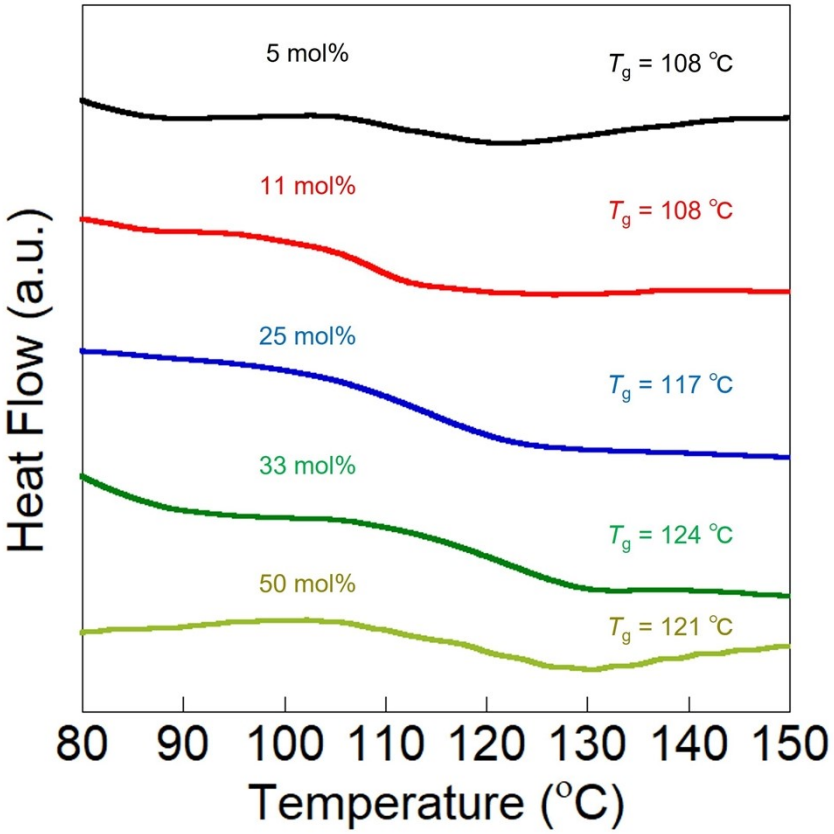


Fig. S9 DSC curve for the different electrolytes.