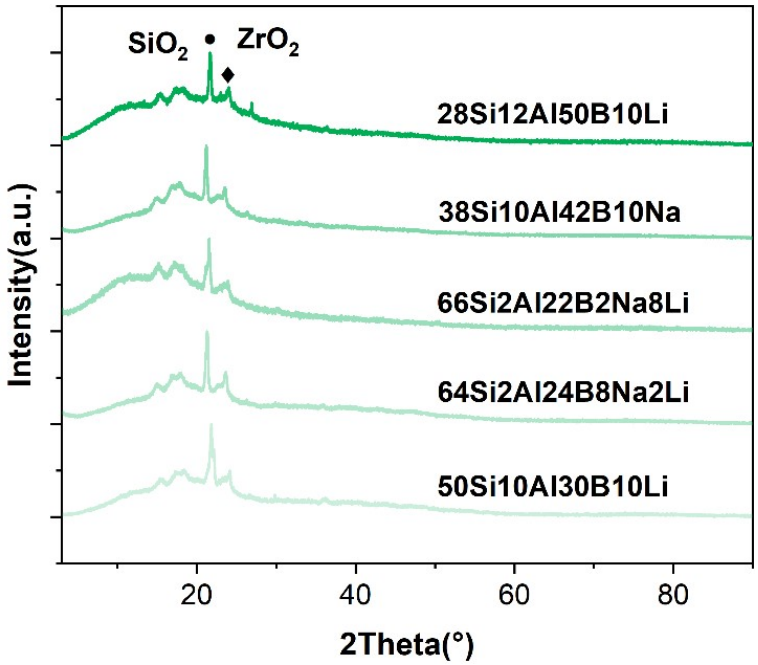
Supplementary information

S1: Five candidates glass information

S-Table 1 Five candidates glass information

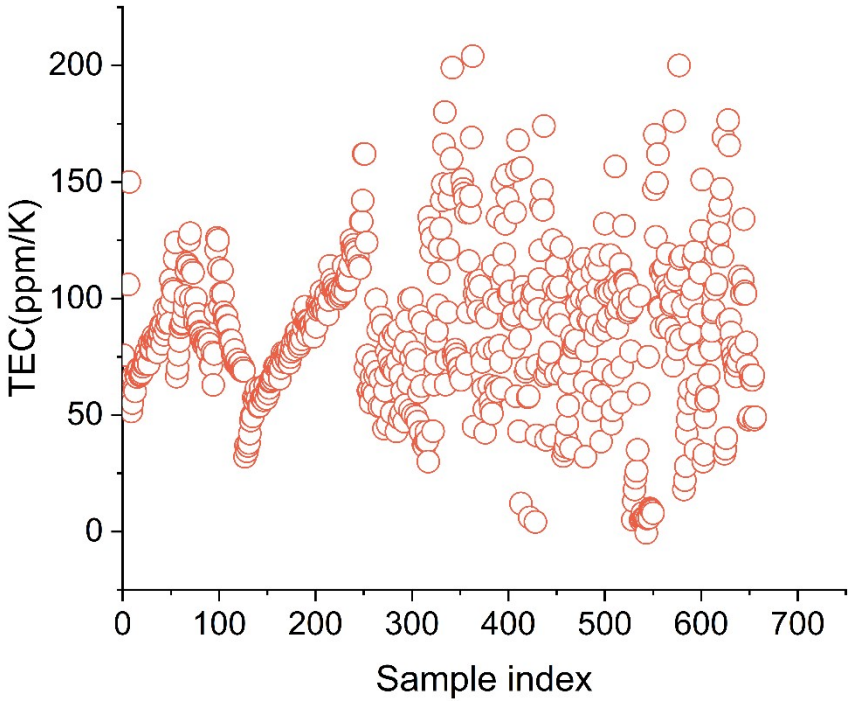
Index	SiO_2	Al_2O_3	B_2O_3	K_2O	Na_2O	Li_2O	Distance	n_c
1	28	12	50	0	0	10	12.95	2.915
2	64	2	24	0	8	2	3.742	3.131
3	66	2	22	0	2	8	3.1544	3.143
4	38	10	42	0	10	0	14.773	2.965
5	50	10	30	0	0	10	0	3.026

S2: XRD pattern of the five potential glass for the matched sealing with Kovar alloy

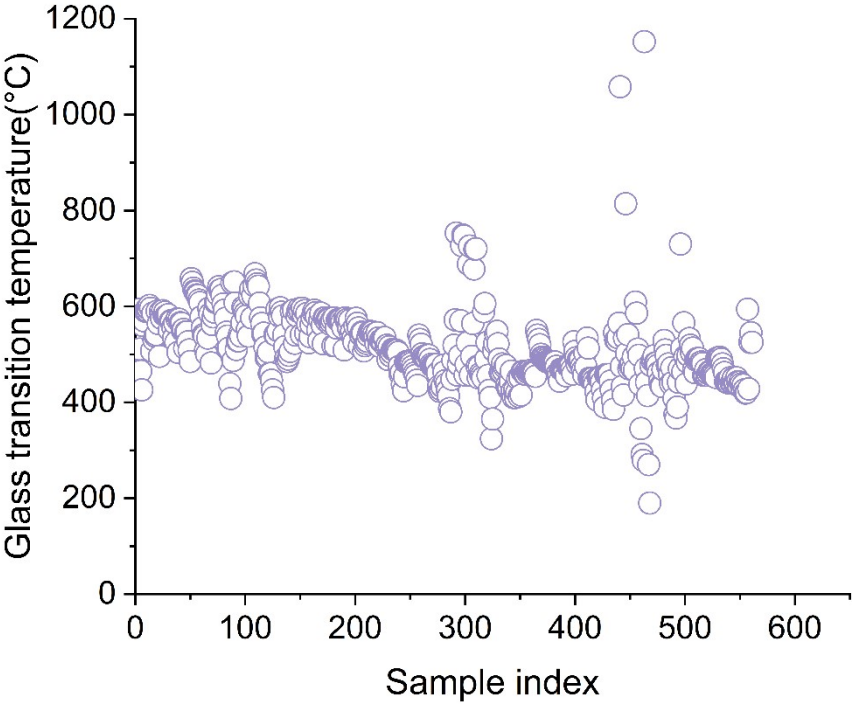


Supplementary Figure 1 XRD pattern of the five potential glass

S3: Raw data analysis



Supplementary Figure 2 TEC distribution of the glasses in the Sciglass dataset



Supplementary Figure 3 Tg distribution of the glasses in the Sciglass dataset

From the distribution of the raw data, it can be observed that the thermal expansion coefficient data is relatively uniformly distributed. The thermal expansion coefficient of the samples range from 0.5~20 ppm/K. Therefore, we believe that the prediction model for the thermal expansion coefficient trained on this data will also achieve good accuracy, which is consistent with our research presented in the main body of the manuscript. In contrast, the distribution of the glass transition temperature data shows that the glass transition temperatures of most glass

compositions are concentrated between 400~600°C. This may result in inherent systematic bias during the training process of the glass transitions with glass transition temperatures between 400°C and 600°C more accurately. However, predictions for glass compositions with significantly higher or lower glass transition temperatures may exhibit considerable errors. If model optimization is required in the future, this will be the primary area for improvement.

S4: Validation analysis outside the Sciglass dataset

We use external data from *Thermal Expansion of Binary Alkali Silicate.* Machine learning model generated through topological constrained theory have demonstrated that the thermal expansion coefficient model can make highly accurate predictions, whether using Sciglass data or external data. However, for the glass transition temperature, it's evident that the uneven distribution of training data has caused significant deviations in the model's performance on external data, which is not characteristic of a good model. Nevertheless, since the glass transition temperature is not a highly important properties in the glass used for our electronic devices, the current level of accuracy still allows us to discover new glass materials.

Supplementary Table 1 Predicted and experimental values of the thermal expansion coefficient model validated with external data

SiO_2	Al_2O_3	B_2O_3	K_2O	Na_2O	Li_2O	TEC_{exp} (10^{-7}/K)	TEC_{pred} (10^{-7}/K)	Deviation (10^{-7}/K)
68	0	0	0	0	32	95.2	109.12	13.925
65.4	0	0	0	0	34.6	99.6	115.73	16.1332
62.1	0	0	0	0	37.9	106.2	123.04	16.8556
60.4	0	0	0	0	39.6	109.5	126.24	16.7405
79.7	0	0	0	20.3	0	97.5	97.31	0.18769
76	0	0	0	24	0	109.7	112.96	3.2636
68.9	0	0	0	31.1	0	136	139.17	3.1719
66.2	0	0	0	33.8	0	143.9	148.93	5.0305
62.8	0	0	0	37.2	0	152.1	159.73	7.6292
82.7	00	0	17.3	0	0	101.2	98.62	2.5751
76.8	0	0	23.2	0	0	129.6	126.97	2.63023
72.2	0	0	27.8	0	0	150	147.92	2.0850
68.2	0	0	31.8	0	0	158.2	165.30	7.0971

Supplementary Table 2 Predicted and experimental values of the glass transition temperature model validated with external data

SiO_2	Al_2O_3	B_2O_3	K_2O	Na_2O	Li_2O	Tg_{exp} (10^{-7}/K)	Tg_{pred} (10^{-7}/K)	Deviation (10^{-7}/K)
68	0	0	0	0	32	498	670.396	172.396

65.4	0	0	0	0	34.6	483	670.409	187.409
62.1	0	0	0	0	37.9	481	670.41	189.41
60.4	0	0	0	0	39.6	477	670.41	193.41
79.7	0	0	0	20.3	0	507	477.169	29.831
76	0	0	0	24	0	503	469.078	33.9218
68.9	0	0	0	31.1	0	490	468.725	21.275
66.2	0	0	0	33.8	0	479	464.8846	14.1154
62.8	0	0	0	37.2	0	467	444.953	22.047
82.7	00	0	17.3	0	0	528	636.1479	108.148
76.8	0	0	23.2	0	0	511	666.7946	155.795
72.2	0	0	27.8	0	0	453	670.1262	217.126
68.2	0	0	31.8	0	0	454	670.3932	216.393

S5: Uncertainty of the machine learning model

Supplementary Table 3 Uncertainty distribution of the thermal expansion coefficient prediction model

ANN	SVM	Tree Decision	Average	Standard deviation
670.3957	542.709	480.8338	564.6462	68.35333
670.4086	545.2884	477.3263	564.3411	69.25476
670.4102	548.5622	457.7323	558.9016	75.45908
670.4102	550.2488	457.7323	559.4638	75.40445
477.169	479.5302	480.3131	479.0041	1.157363
469.0782	473.8012	467.2676	470.049	2.38525
468.725	462.8076	471.2846	467.6057	3.07445
464.8846	458.627	469.1697	464.2271	3.749092
444.953	453.3625	444.3311	447.5489	3.566894
636.1479	528.1254	483.6686	549.314	55.44907
666.7946	533.9787	475.0758	558.6164	69.44166
670.1262	538.5422	482.6594	563.7759	68.05699
670.3932	542.5106	480.8338	564.5792	68.36835

Supplementary Table 4 Supplementary Table 3 Uncertainty distribution of glass transition temperature prediction model

XGBoot	LinearRegreesion	SVM	Tree Decision	Average	Standard deviation
109.125	110.3961	105.9034	107.08	108.1261	1.745371
115.7332	118.7028	113.3551	117.5833	116.3436	2.025257
123.0356	128.7688	122.654	180.75	138.8021	24.33945

126.2405	133.099	127.3748	180.75	141.8661	22.59965
97.31231	97.21065	98.1323	95.9648	97.15501	0.774521
112.9636	112.119	113.1646	111.3238	112.3928	0.731311
139.1719	142.1259	140.3559	148.8333	142.6218	3.737129
148.9305	153.3548	150.1253	140.4875	148.2245	4.751114
159.7292	167.0155	161.9799	168.3292	164.2634	3.531222
98.6249	96.1773	99.5326	87.15	95.3712	4.902594
126.9698	124.9929	128.1305	141.7778	130.4677	6.625513
147.915	146.7902	149.1597	162.3714	151.5591	6.298509
165.2971	165.592	166.5431	162.3714	164.9509	1.558826