Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supplemental information for "$B_2O_3/SiO_2$ substitution effect on structure and properties of $Na_2O$-CaO-SrO-$P_2O_5$-$SiO_2$ bioactive glasses from molecular dynamics simulations"

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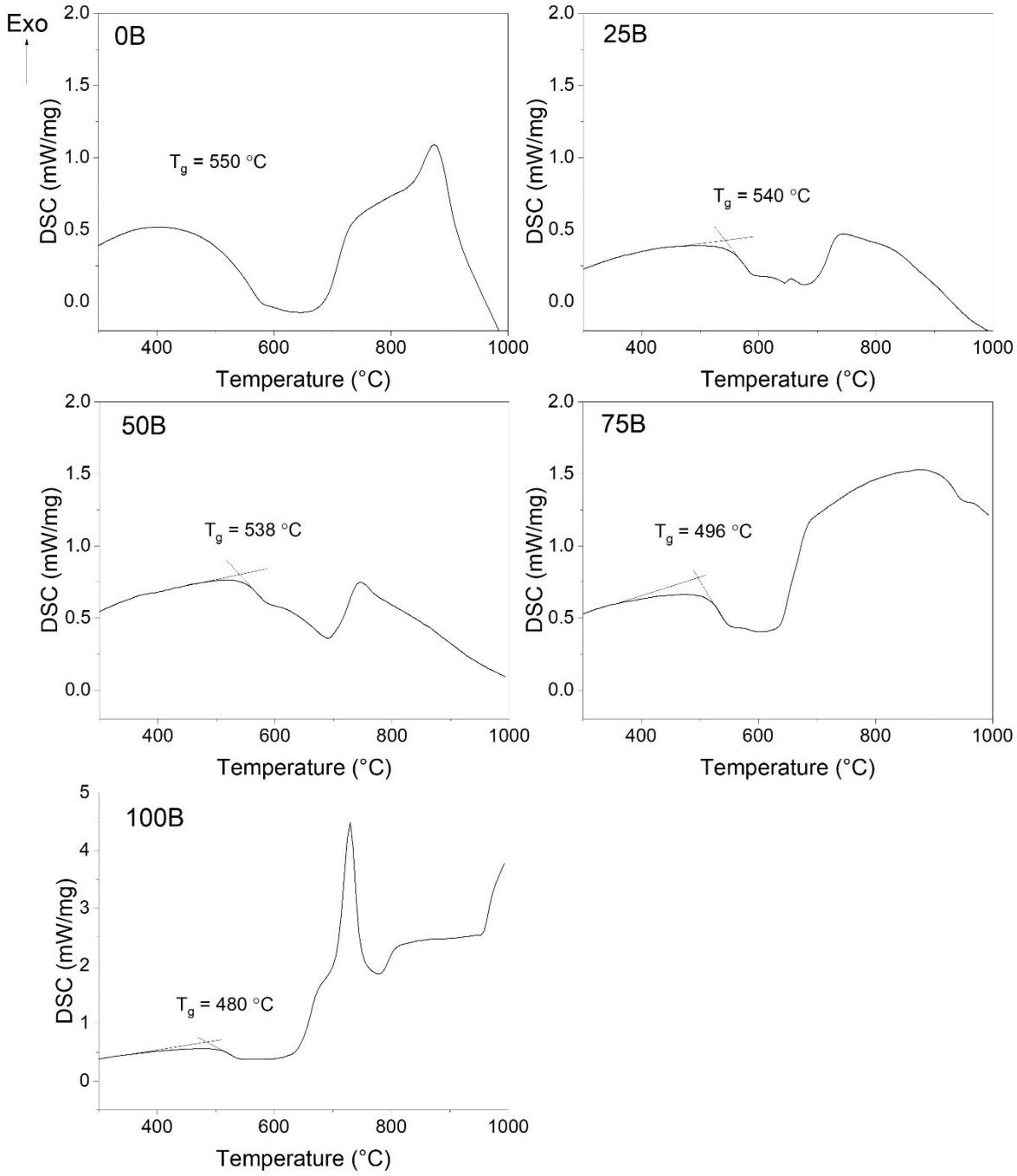


Fig. S1 DSC curves with a heating rate of 20 ˚C/min for different samples

The $T_g$ for sample 0B was determined from the first minimum peak position of the first-order derivative curve of DSC

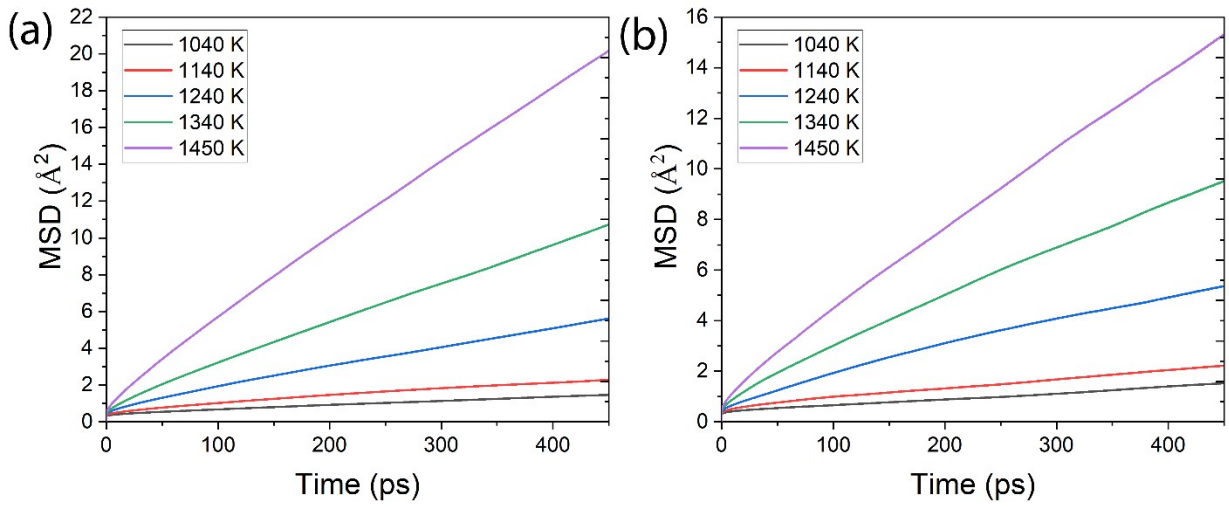


Fig. S2 Low temperature range (1040-1450 K) linear MSDs for (a) Ca and (b) Sr

Table S1 Diffusion coeffcients ($10^{-6}$ cm$^2$/s) of Ca in low temoperature range

| T (K) | 0B | 25B | 50B | 75B | 100B |
|---|---|---|---|---|---|
| 1040 | 0.047 ± 0.013 | 0.057 ± 0.009 | 0.028 ± 0.004 | 0.064 ± 0.011 | 0.074 ± 0.023 |
| 1140 | 0.063 ± 0.007 | 0.073 ± 0.027 | 0.062 ± 0.004 | 0.108 ± 0.016 | 0.087 ± 0.017 |
| 1240 | 0.121 ± 0.038 | 0.114 ± 0.050 | 0.143 ± 0.026 | 0.177 ± 0.057 | 0.277 ± 0.034 |
| 1340 | 0.181 ± 0.032 | 0.223 ± 0.060 | 0.363 ± 0.042 | 0.507 ± 0.031 | 0.712 ± 0.058 |
| 1450 | 0.361 ± 0.041 | 0.423 ± 0.052 | 0.692 ± 0.036 | 1.200 ± 0.214 | 1.687 ± 0.098 |

Table S2 Diffusion coeffcients ($10^{-6}$ cm$^2$/s) of Sr in low temoperature range

| T (K) | 0B | 25B | 50B | 75B | 100B |
|---|---|---|---|---|---|
| 1040 | 0.037 ± 0.006 | 0.053 ± 0.017 | 0.033 ± 0.010 | 0.545 ± 0.020 | 0.045 ± 0.019 |
| 1140 | 0.031 ± 0.016 | 0.084 ± 0.013 | 0.066 ± 0.016 | 0.704 ± 0.017 | 0.063 ± 0.006 |
| 1240 | 0.097 ± 0.026 | 0.100 ± 0.061 | 0.107 ± 0.042 | 0.146 ± 0.025 | 0.237 ± 0.052 |
| 1340 | 0.147 ± 0.020 | 0.230 ± 0.054 | 0.267 ± 0.042 | 0.407 ± 0.037 | 0.595 ± 0.055 |
| 1450 | 0.278 ± 0.104 | 0.409 ± 0.042 | 0.670 ± 0.134 | 1.001 ± 0.041 | 1.384 ± 0.094 |

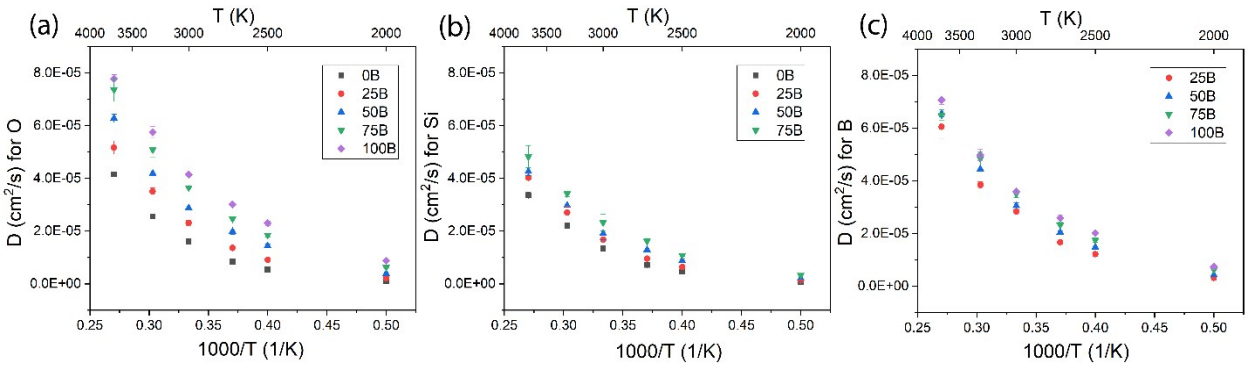


Fig. S3 High temperature range (2000-3700 K) diffusion coefficients (non-logarithm scale) for (a) O (b) Si (c) B calculated from MD simulations