# Supplemetary materials to Ionic Self-Diffusion and the Glass Transition Anomaly in Aluminosilicates

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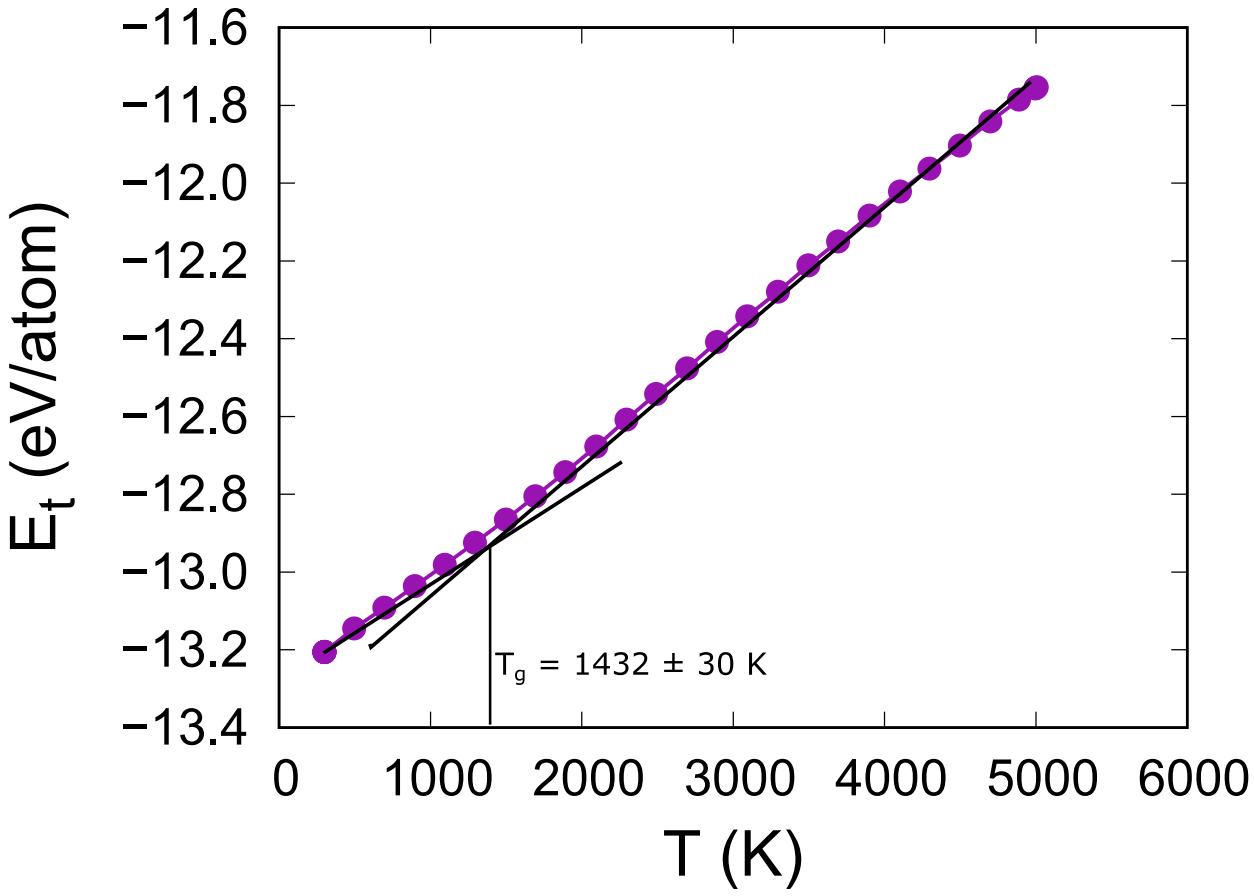


FIG. S1. Total energy ($E_t$) as a function of the temperature in NaAS system during the cooling process. Black lines are for linear fitting.

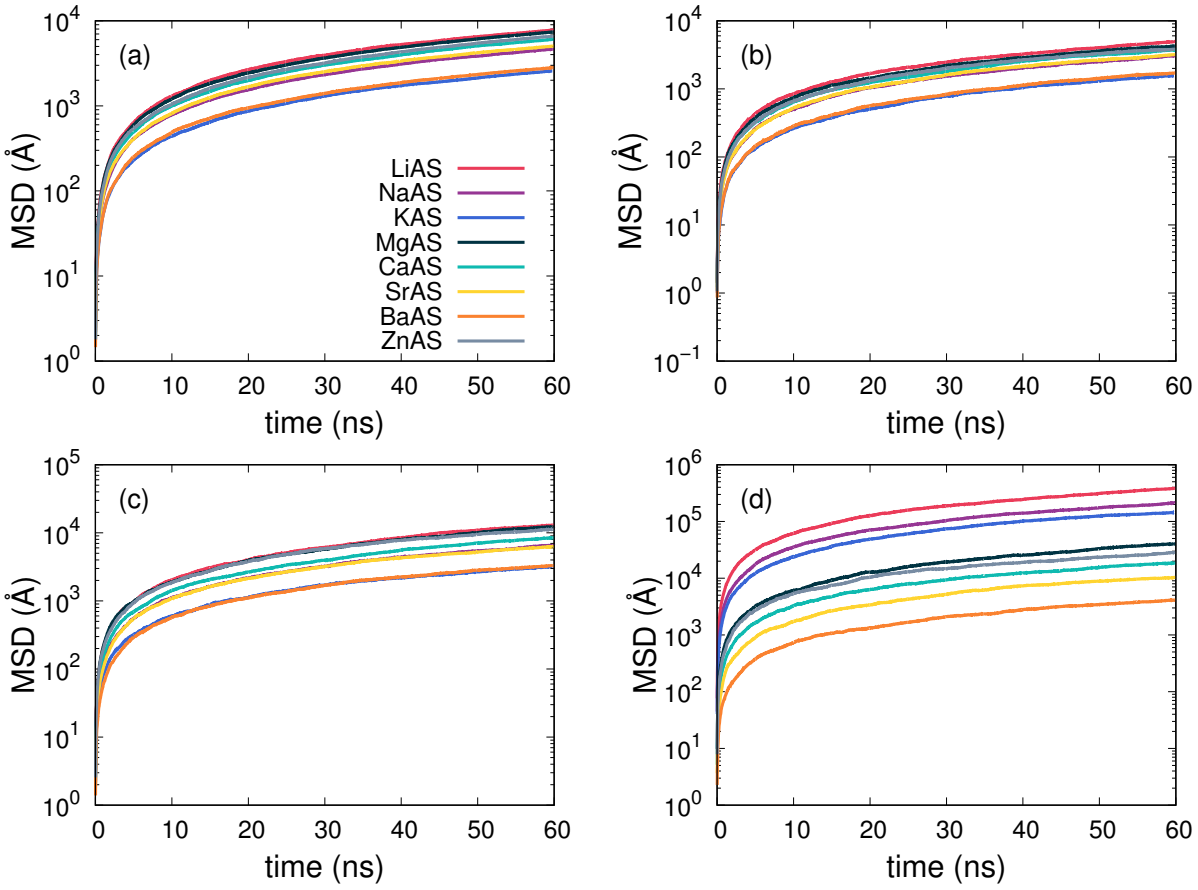


FIG. S2. Mean squared displacement of O, Si, Al, and X (X = Li, Na, K, Mg, Ca, Sr, Ba, and Zn) at 1900 K for the studied aluminosilicate glasses.

TABLE S1. Diffusion activation energy barrier $E_a$(eV) for all elements in our glasses.

| System | $FS$ (Å$^{-2}$) | $E_{a_{Si}}$ | $E_{a_{Al}}$ | $E_{a_O}$ | $E_{a_X}$ |
|---|---|---|---|---|---|
| $LiAS$ | 1.49 | 1.36 ± 0.04 | 1.16 ± 0.04 | 1.28 ± 0.04 | 0.48 ± 0.02 |
| $NaAS$ | 0.69 | 1.54 ± 0.02 | 1.42 ± 0.04 | 1.47 ± 0.05 | 0.57 ± 0.01 |
| $KAS$ | 0.39 | 1.79 ± 0.07 | 1.61 ± 0.09 | 1.69 ± 0.07 | 0.59 ± 0.02 |
| $MgAS$ | 3.12 | 1.43 ± 0.04 | 1.17 ± 0.05 | 1.30 ± 0.05 | 0.92 ± 0.05 |
| $CaAS$ | 1.51 | 1.45 ± 0.08 | 1.28 ± 0.05 | 1.38 ± 0.05 | 1.11 ± 0.05 |
| $SrAS$ | 1.13 | 1.51 ± 0.06 | 1.37 ± 0.07 | 1.44 ± 0.06 | 1.25 ± 0.07 |
| $BaAS$ | 0.89 | 1.70 ± 0.09 | 1.60 ± 0.09 | 1.63 ± 0.08 | 1.53 ± 0.11 |
| $ZnAS$ | 3.12 | 1.45 ± 0.04 | 1.20 ± 0.03 | 1.34 ± 0.05 | 1.02 ± 0.05 |

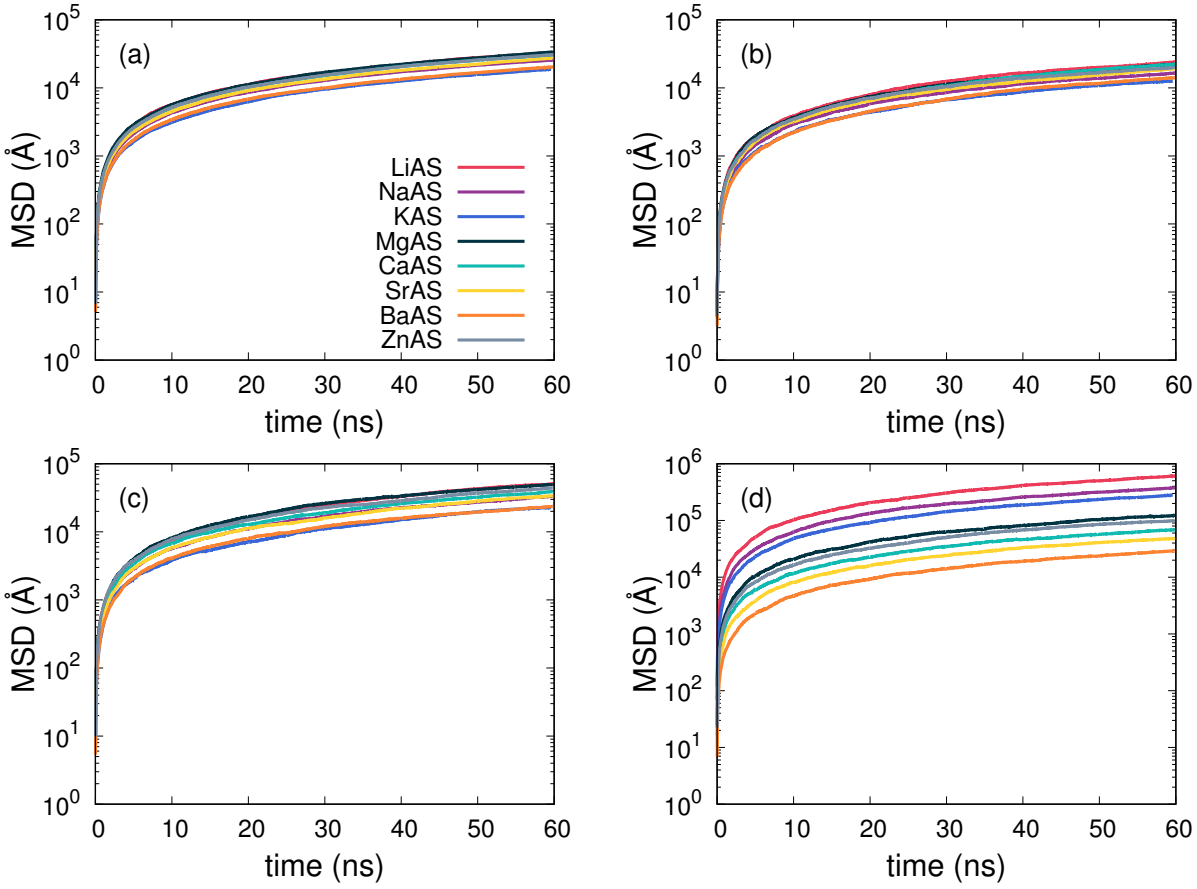


FIG. S3. Mean squared displacement of O, Si, Al, and X (X = Li, Na, K, Mg, Ca, Sr, Ba, and Zn) at 2300 K for the studied aluminosilicate glasses.

TABLE S2. Diffusion pre-exponential factor $lnD_0(\mathrm{m}^2.\mathrm{s}^{-1})$ for all elements in our glasses.

| System | $FS$ (Å$^{-2}$) | $D_{0_{Si}}$ | $D_{0_{Al}}$ | $D_{0_O}$ | $D_{0_X}$ |
|---|---|---|---|---|---|
| $LiAS$ | 1.49 | -14.35 ± 0.20 | -14.61 ± 0.21 | -14.38 ± 0.19 | -15.46 ± 0.08 |
| $NaAS$ | 0.69 | -13.78 ± 0.10 | -13.72 ± 0.20 | -13.70 ± 0.23 | -15.49 ± 0.06 |
| $KAS$ | 0.39 | -12.82 ± 0.38 | -13.18 ± 0.43 | -12.96 ± 0.35 | -15.68 ± 0.09 |
| $MgAS$ | 3.12 | -14.10 ± 0.24 | -14.61 ± 0.24 | -14.29 ± 0.24 | -14.93 ± 0.25 |
| $CaAS$ | 1.51 | -14.04 ± 0.40 | -14.30 ± 0.26 | -14.00 ± 0.22 | -14.58 ± 0.22 |
| $SrAS$ | 1.13 | -13.85 ± 0.29 | -13.98 ± 0.37 | -13.85 ± 0.28 | -14.25 ± 0.33 |
| $BaAS$ | 0.89 | -13.25 ± 0.47 | -13.21 ± 0.49 | -13.22 ± 0.40 | -13.43 ± 0.52 |
| $ZnAS$ | 3.12 | -14.08 ± 0.23 | -14.50 ± 0.14 | -14.21 ± 0.24 | -14.64 ± 0.27 |

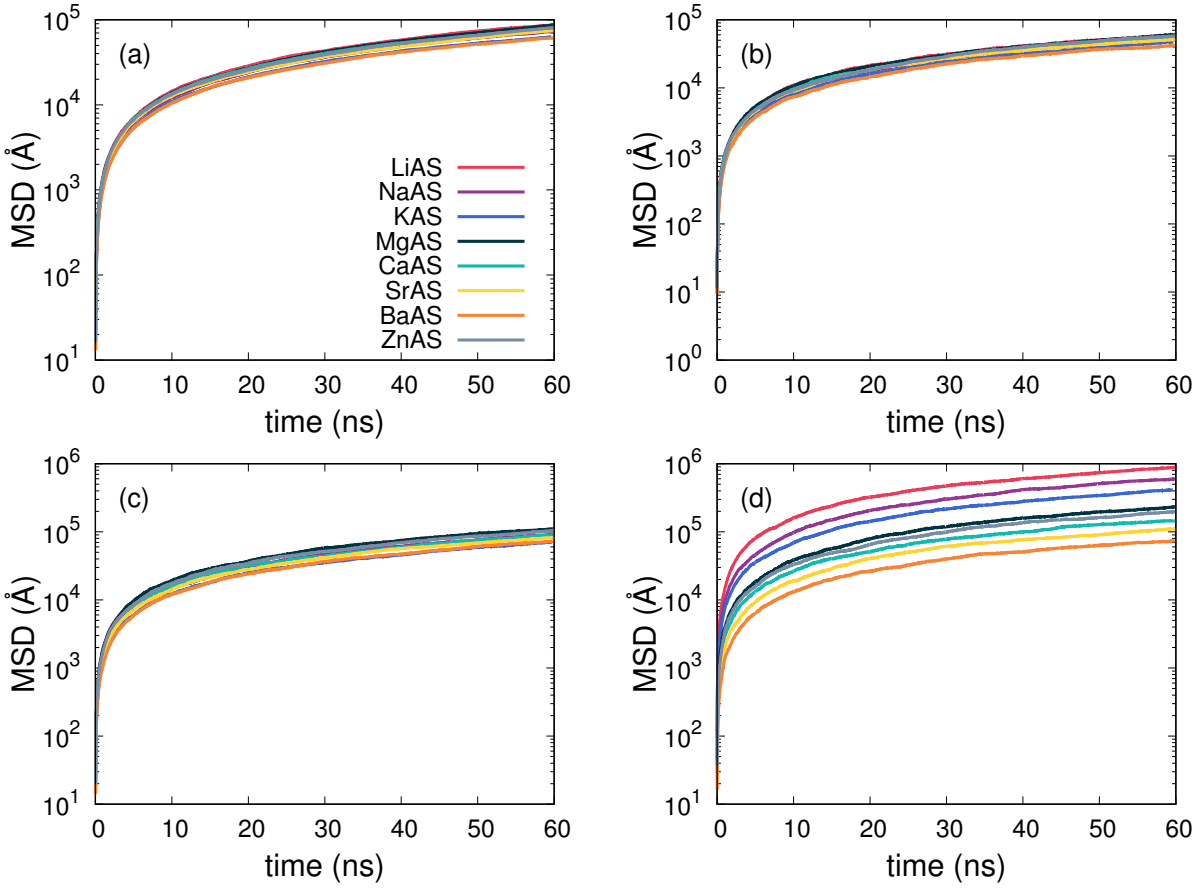


FIG. S4. Mean squared displacement of O, Si, Al, and X (X = Li, Na, K, Mg, Ca, Sr, Ba, and Zn) at 2700 K for the studied aluminosilicate glasses.

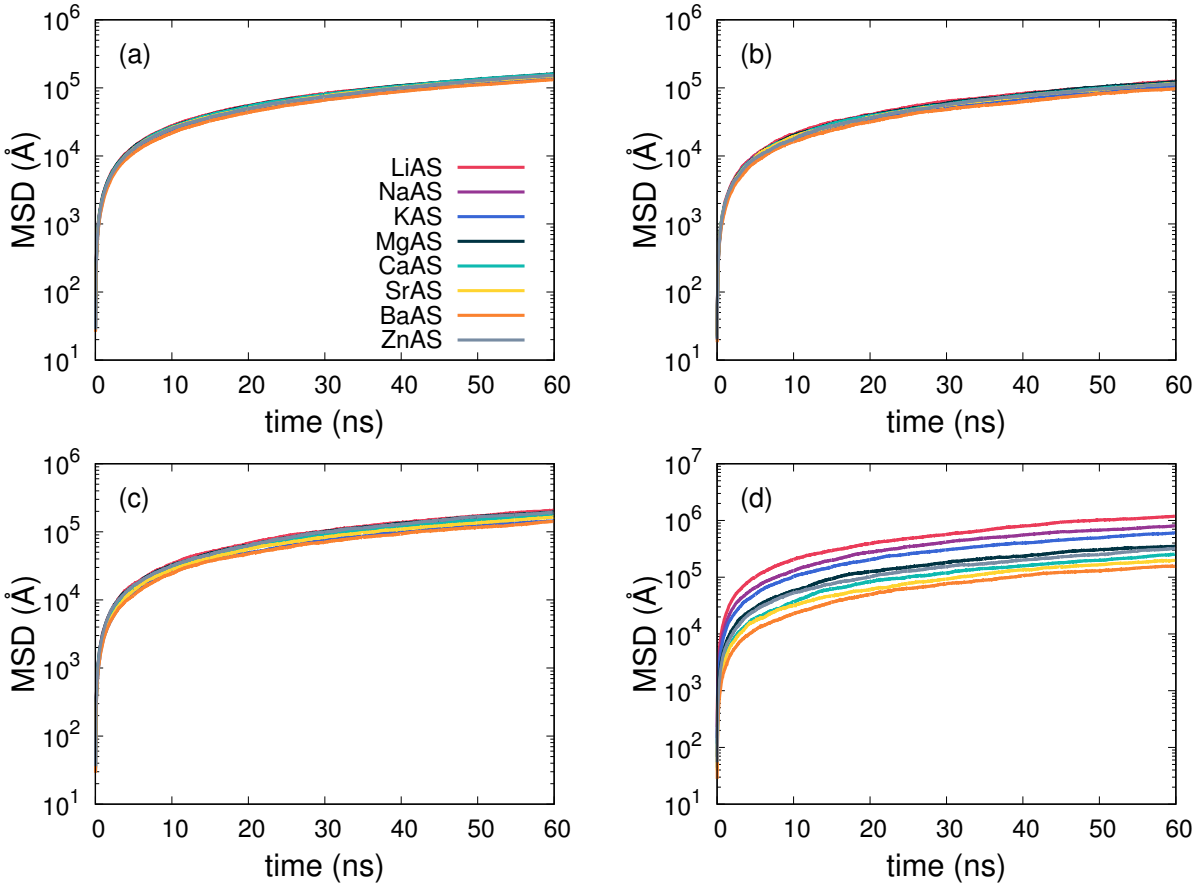


FIG. S5. Mean squared displacement of O, Si, Al, and X (X = Li, Na, K, Mg, Ca, Sr, Ba, and Zn) at 3100 K for the studied aluminosilicate glasses.

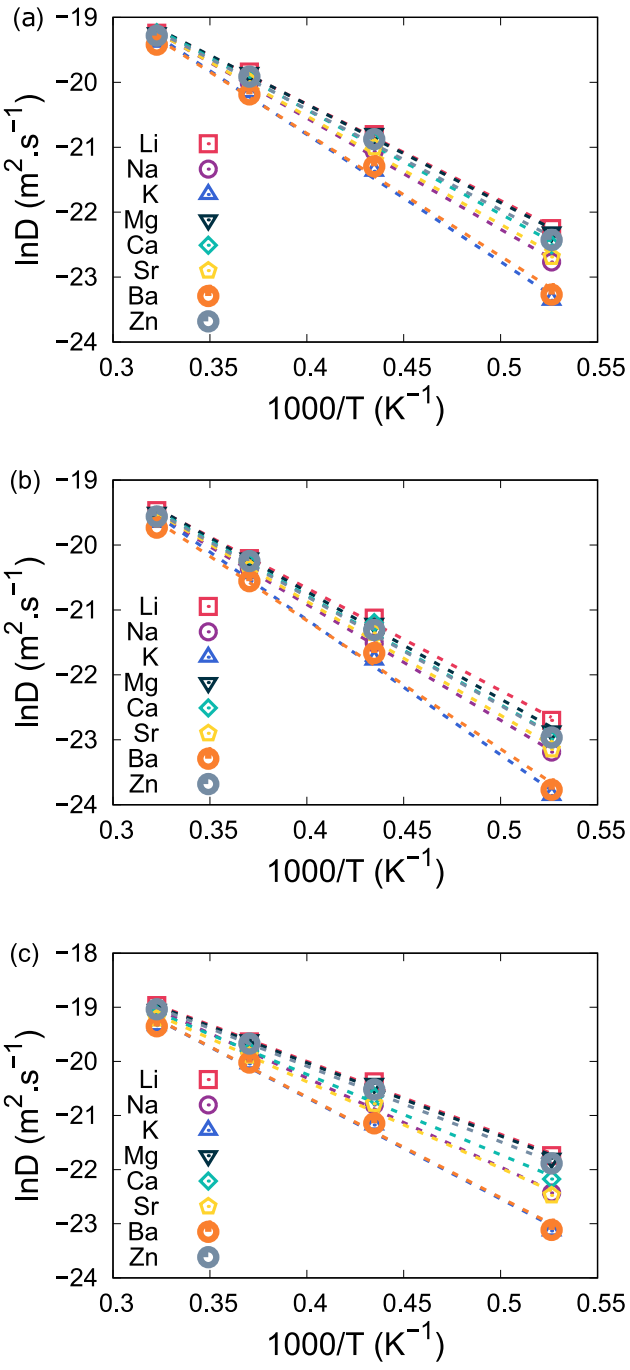


FIG. S6. Diffusion coefficients of (a) O, (b) Si, (c) Al as a function of temperature for the studied aluminosilicate glasses. The symbols represent the simulated data points and the lines are fitted to the Arrhenius law.

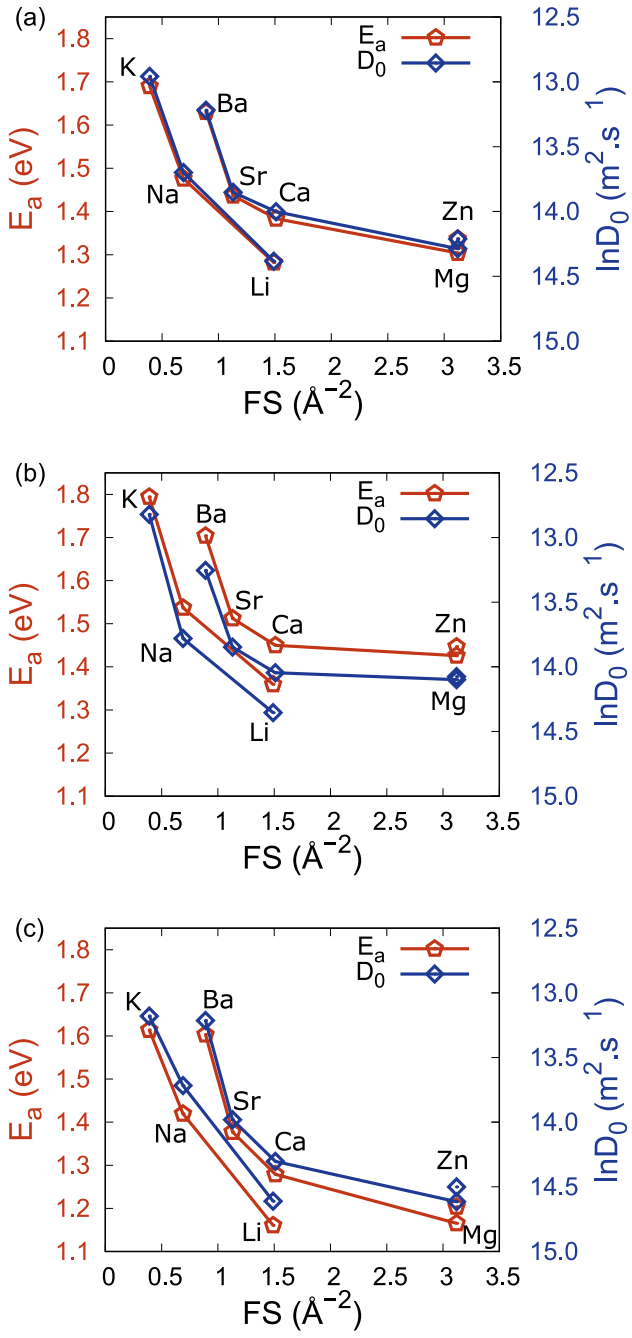


FIG. S7. Activation energies barriers for diffusion $E_a$ and pre-exponential factor $D_0$ of (a) O, (b) Si, and (c) Al, as a function of charge balancing cations field strength for the studied aluminosilicate glasses. The symbols represent the simulated data points and the lines are guide to the eye.

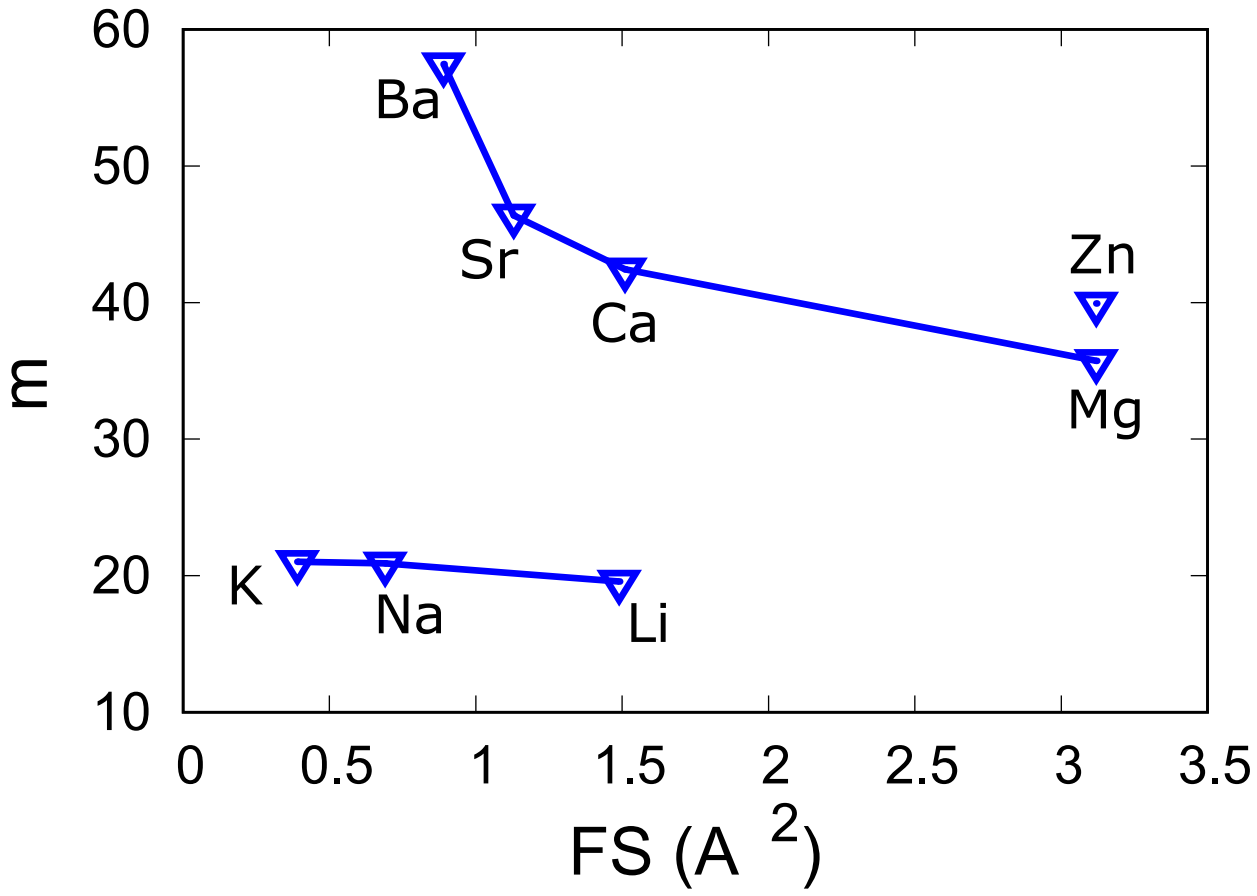


FIG. S8. The fragility index m as a function of FS in the studied aluminosilicate glasses calculated from the Arrhenius behavior. The symbols represent the simulated data points and the lines are guide to the eye.

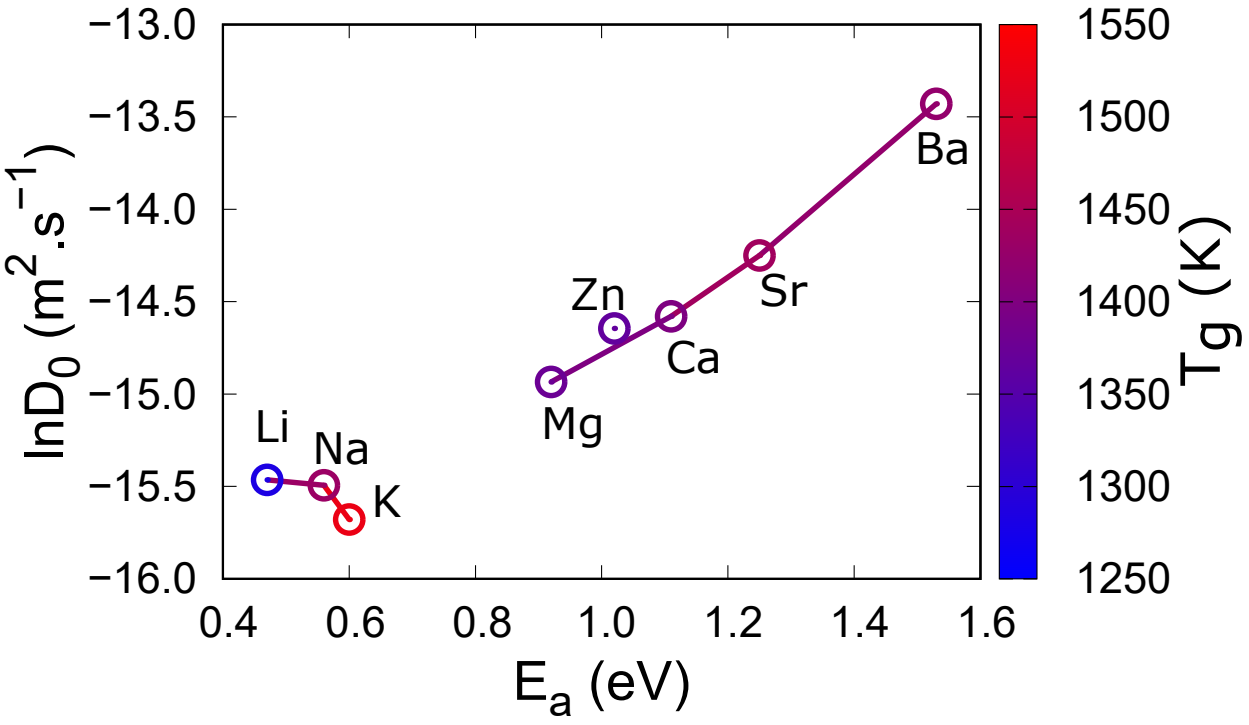


FIG. S9. Pre-exponential factor $D_0$ as a function of the activation energies barriers and $T_g$ for the studied aluminosilicate glasses. The symbols represent the simulated data points and the lines are guide to the eye.