Supporting Information

Ab Initio Modeling of Structure and Properties of Single and Mixed Alkali Silicate Glasses

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This supporting information present the Figures for the 30% doping similar to the 20% doping in the main text.

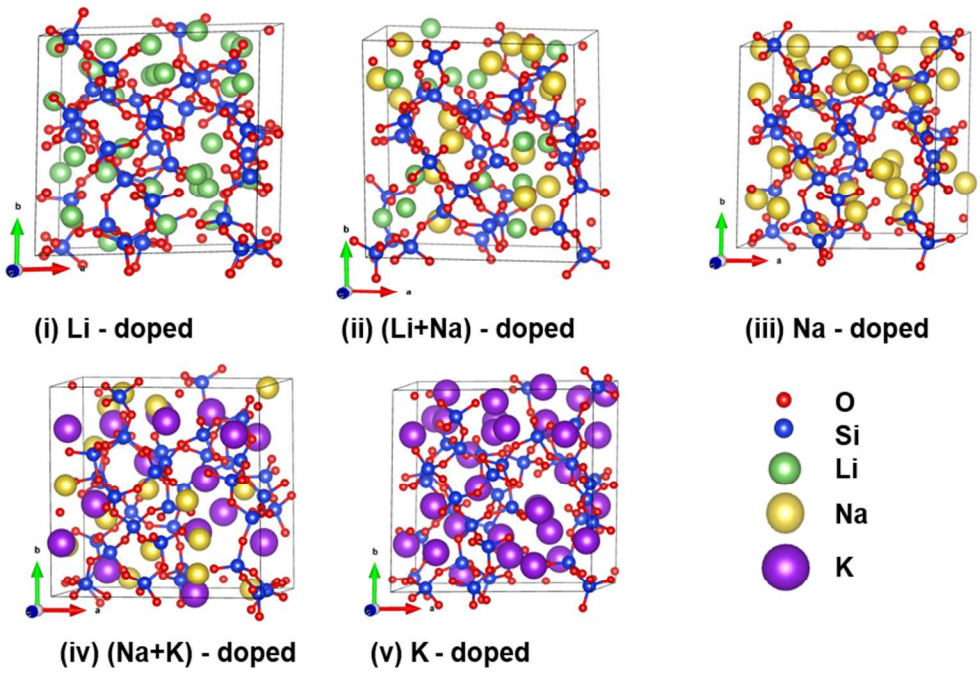

Figure S1: Ball and stick figures of 30 mol. % alkali oxide doped silicate glasses.

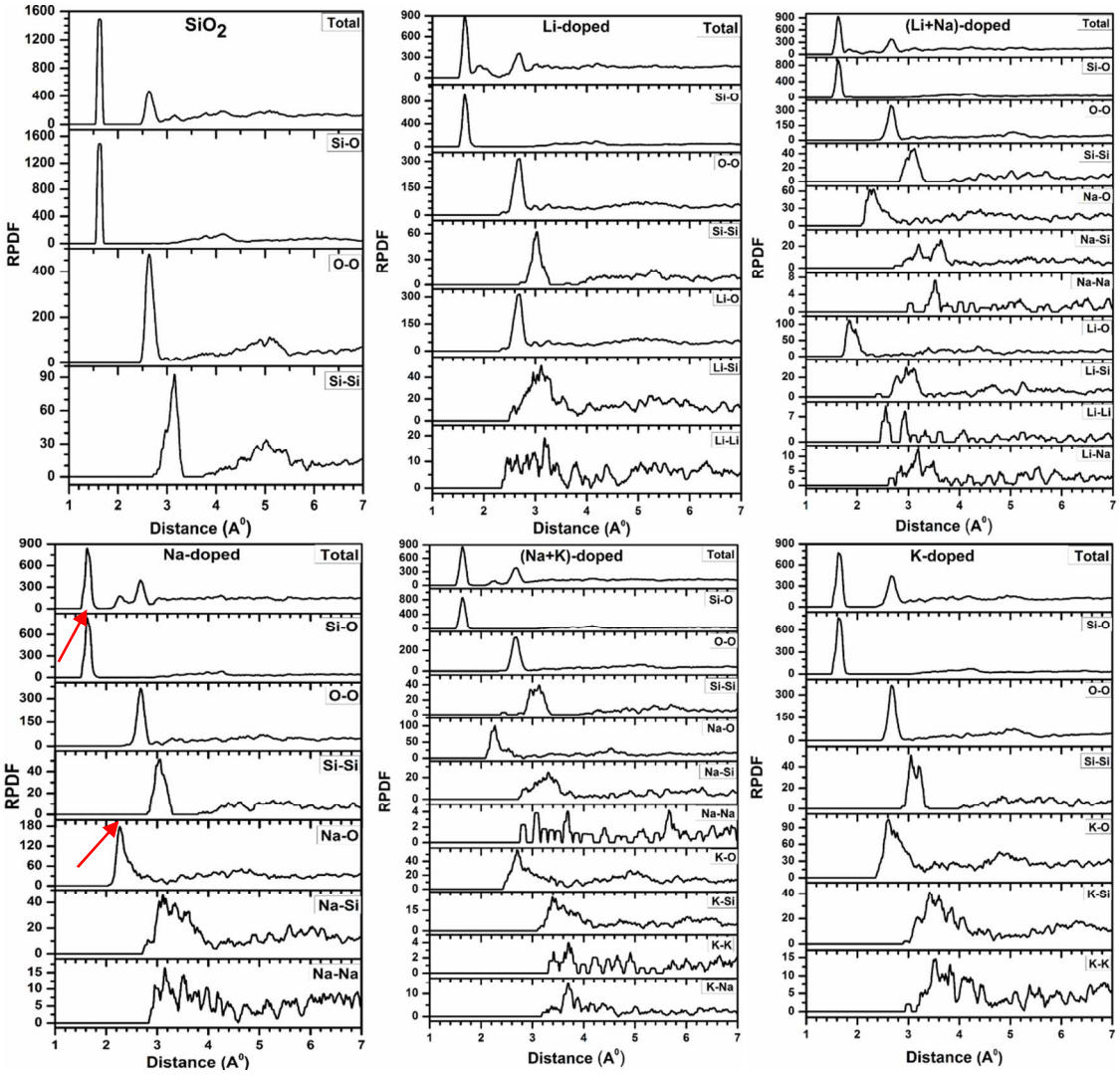

Figure S2: Radial pair distribution functions for 30 mol. % alkali oxide doped silicate glasses. The arrow in the Na-doped panel indicates the position of the experimental (33.33 mol. %) peak from ref. [28].

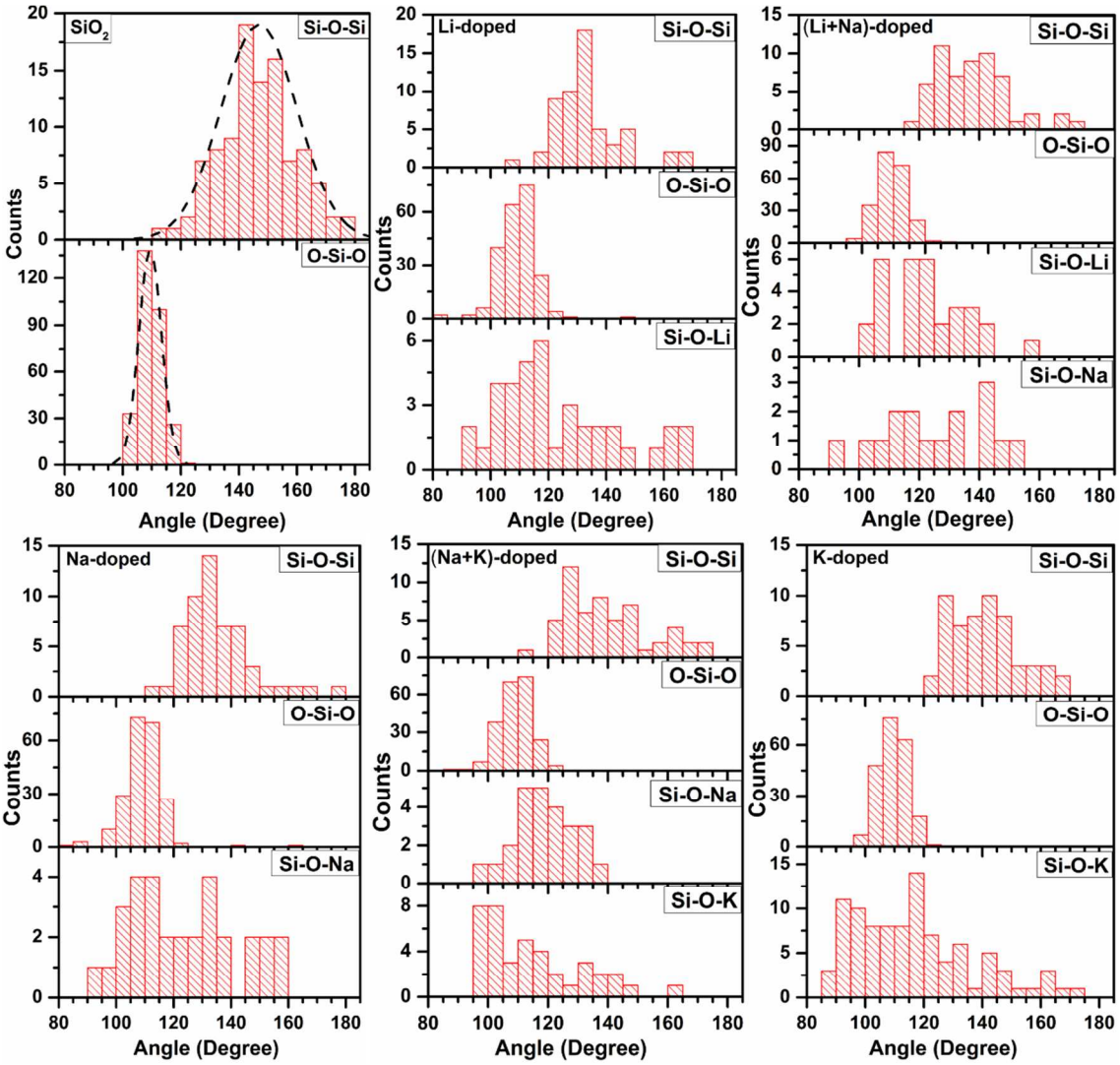

Figure S3: Bond angle distribution for 30 mol. % alkali oxide mixed silicate glasses.

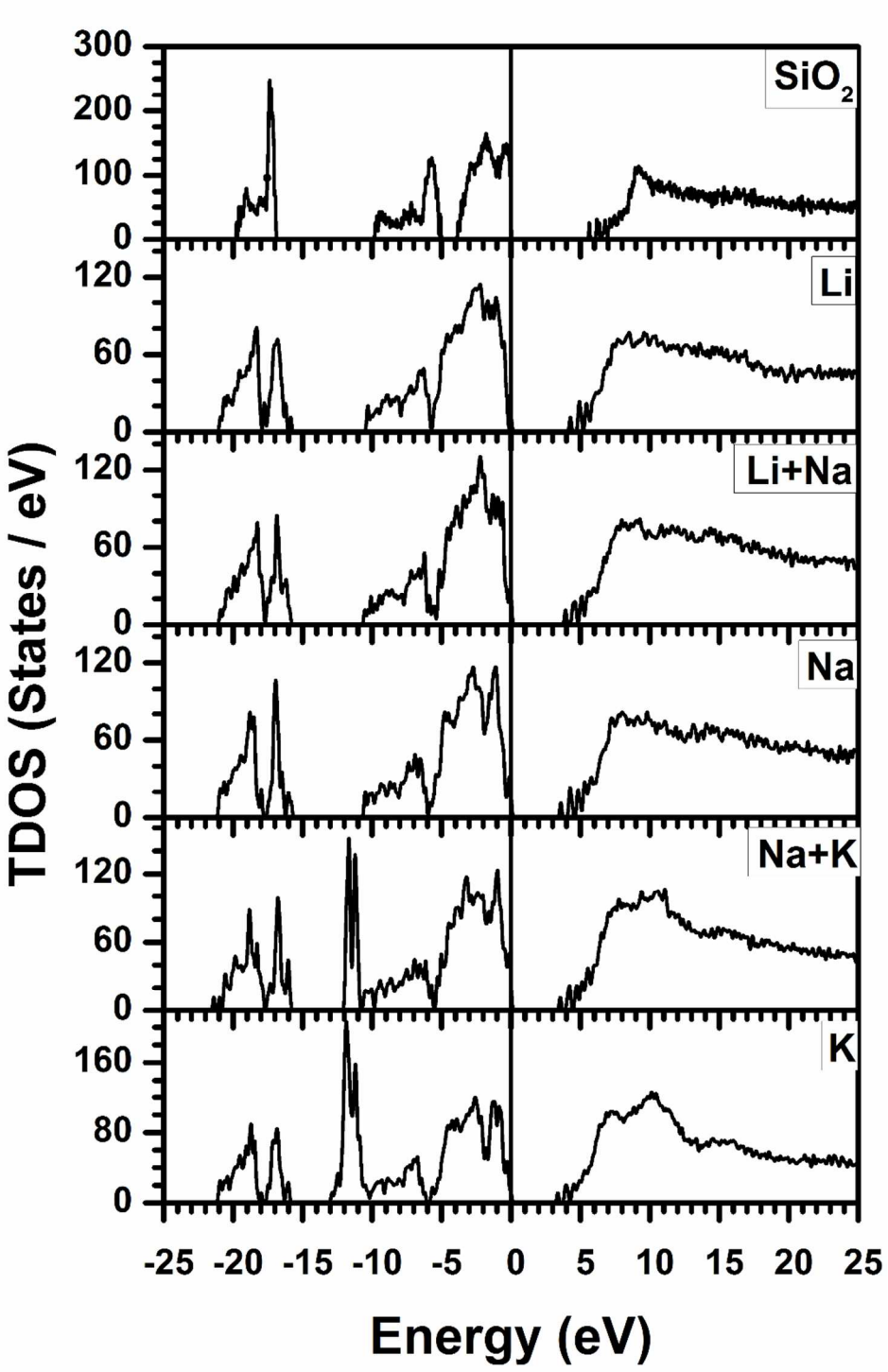

Figure S4: Electronic total density of states for 30 mol. % alkali oxide added silicate glasses.

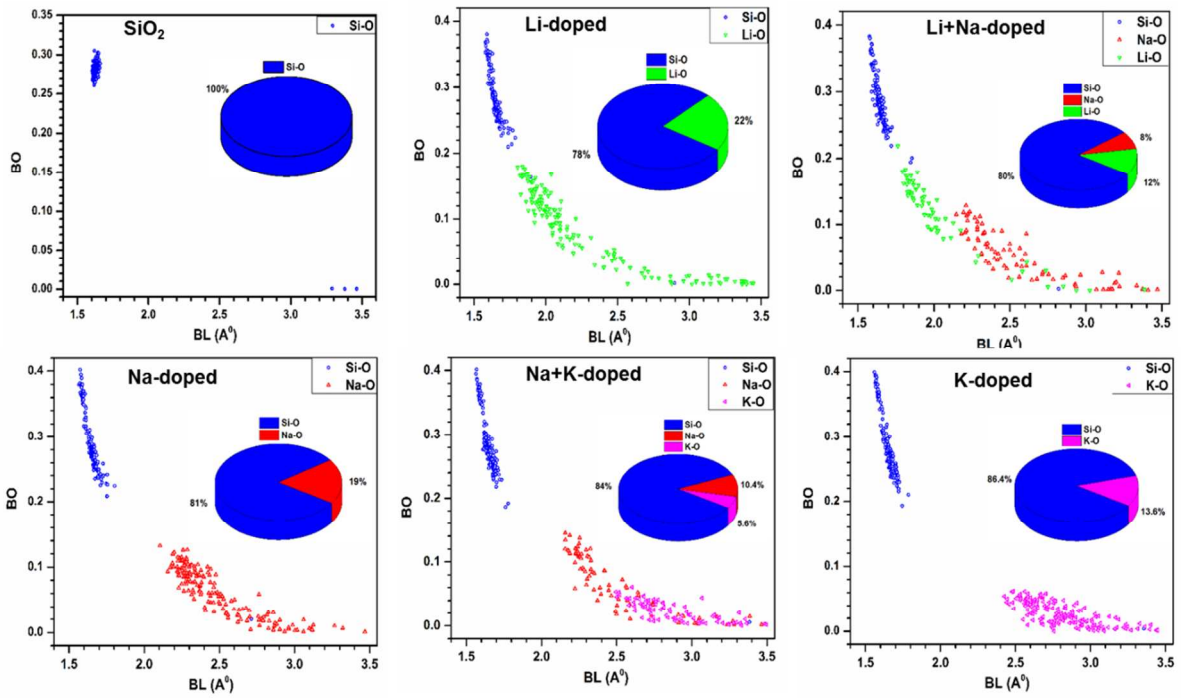

Figure S5: Distribution of bond order versus bond length for 30 mol. % alkali oxide doped glasses.

Inset shows the contribution form different types of bonds.

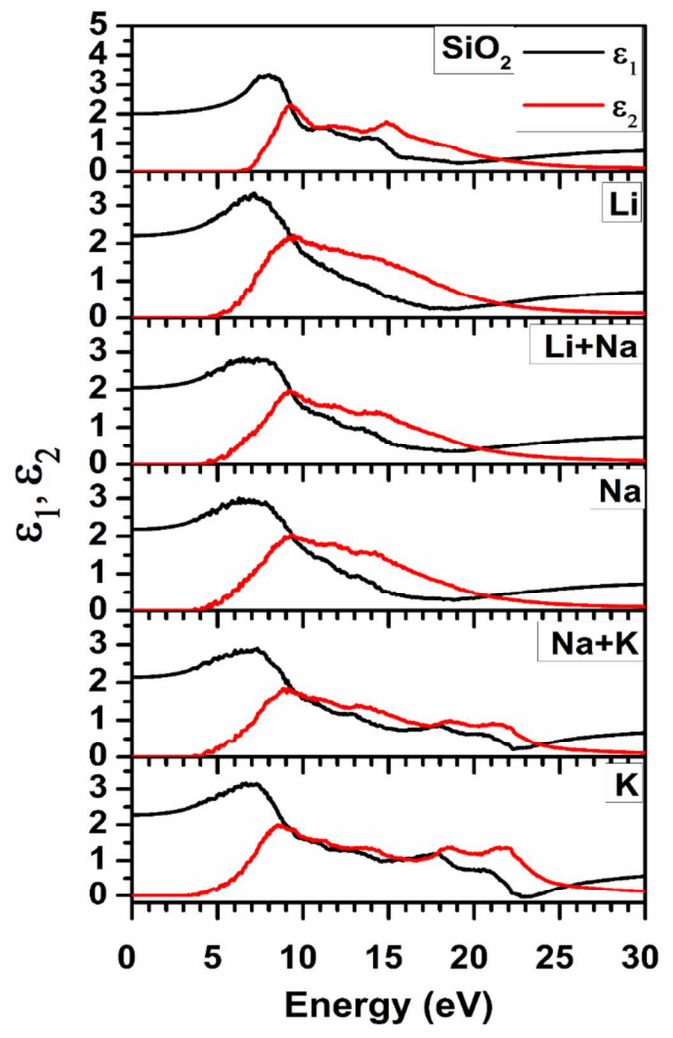

Figure S6: Calculated dielectric constants for the 30 mol. % alkali oxide doped glasses.