Multi-Composition-EPSR: Towards Transferable Potentials To Model Chalcogenide Glass Structures.

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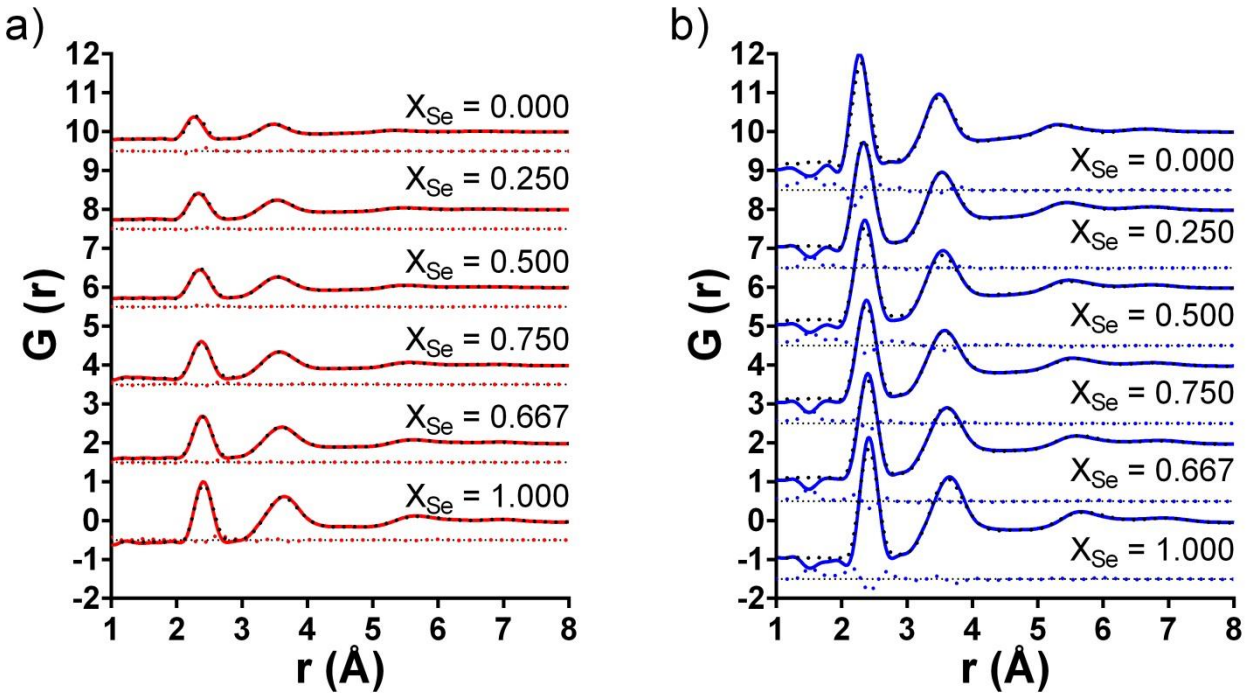

Figure S1: Experimental a) neutron (solid red) and b) X-ray (solid blue) radial distribution functions, G(r), plotted with those produced from the T-EPSR simulations (black dotted lines) for each of the As-S-Se glasses studied. The residuals are shown using coloured dotted lines and these data are shifted to aid clarity.

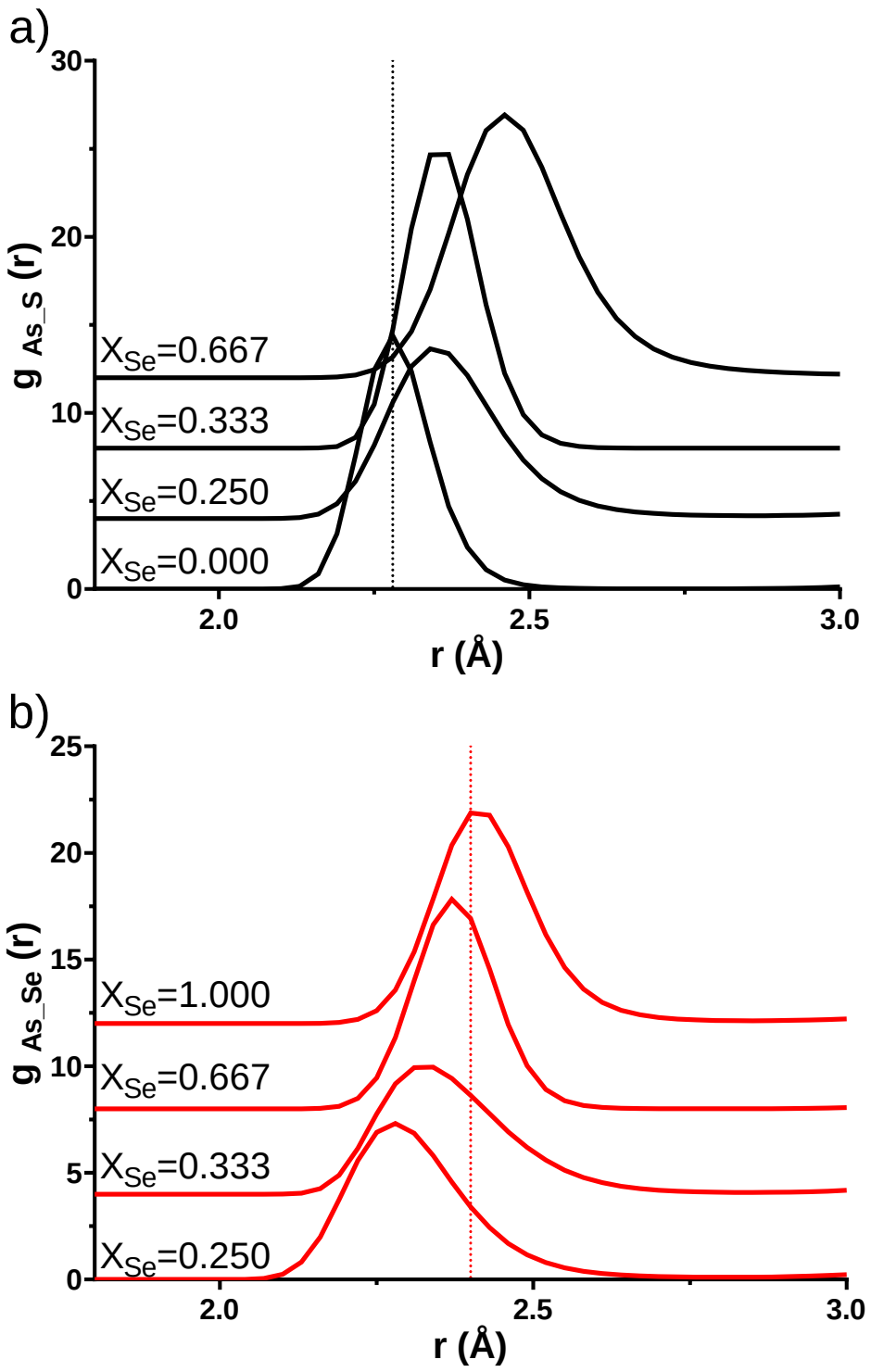

Figure S2**:** Partial radial distribution functions, $g_{As\text{-}Ch}(r)$, for a) arsenic-sulphur (black) and b) arsenic-selenium (red) taken from the T-EPSR simulations of As-S-Se glasses studied. The dotted lines indicate the expected position of the peak as calculated using bond valence.

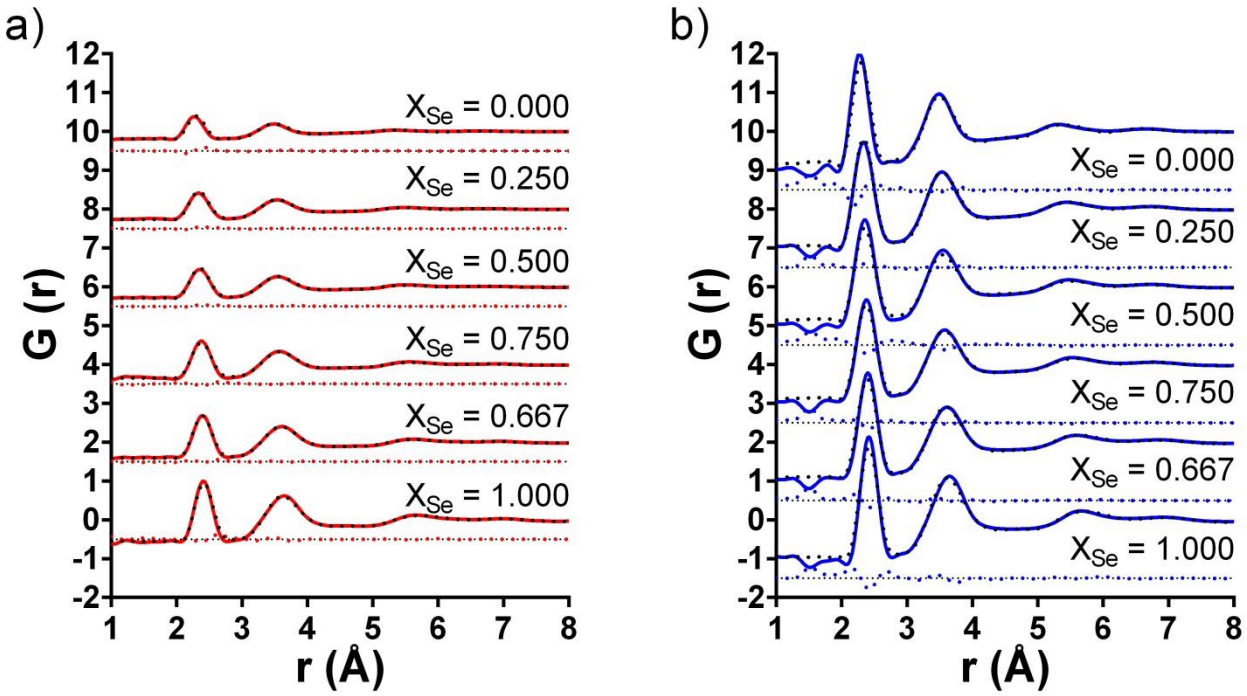

Figure S3: Experimental a) neutron (solid red) and b) X-ray (solid blue) radial distribution functions, G(r), plotted with those produced from the MC-EPSR simulations without Lone Pair atoms (black dotted lines) for each of the As-S-Se glasses studied. The residuals are shown using coloured dotted lines and these data are shifted to aid clarity.

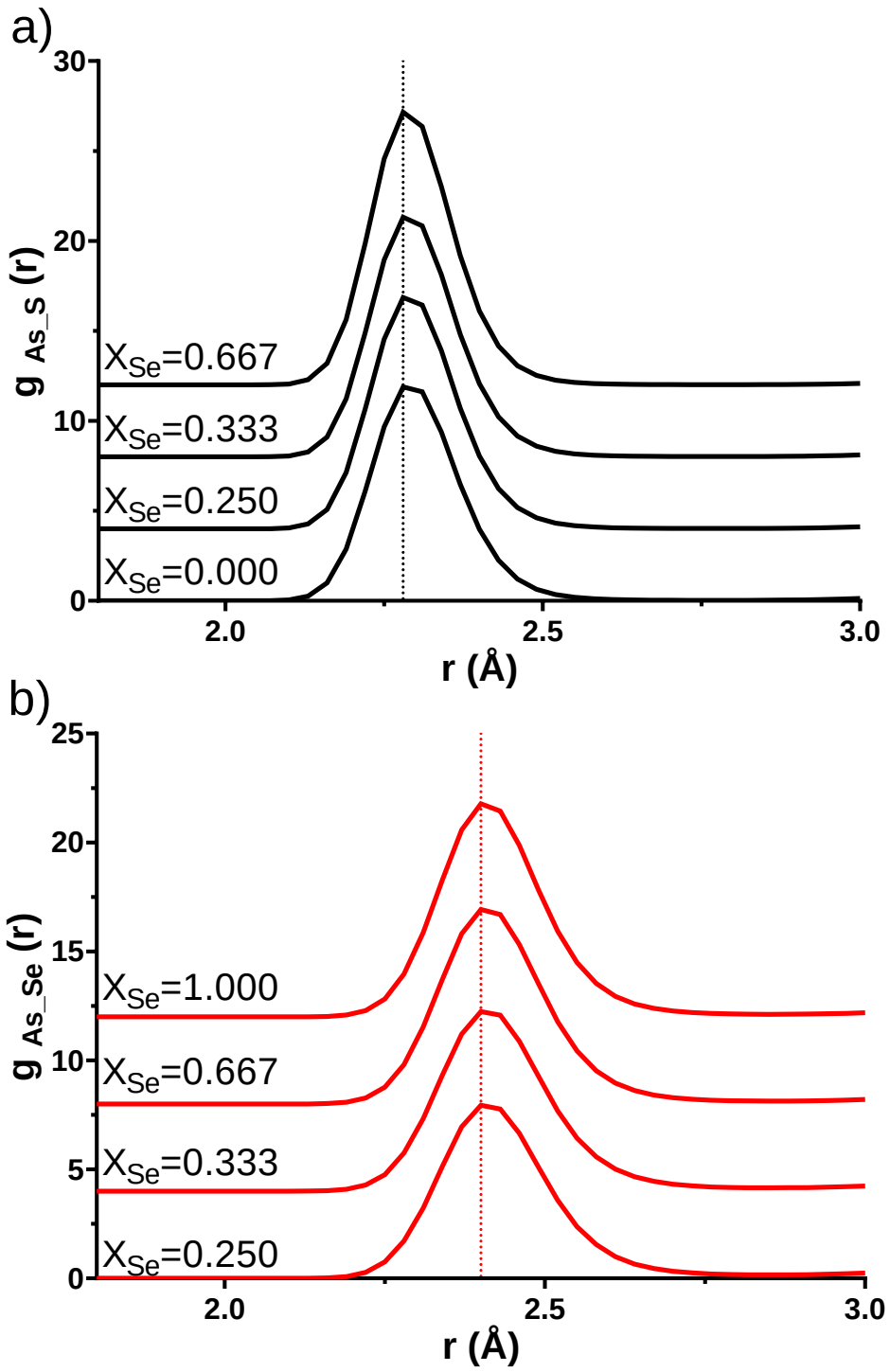

Figure S4: Partial radial distribution functions, $g_{As\text{-}Ch}(r)$, for a) arsenic-sulphur (black) and b) arsenic-selenium (red) taken from the MC-EPSR simulations without Lone Pair atoms for each of the As-S-Se glasses studied. The dotted lines indicate the expected position of the peak as calculated using bond valence.

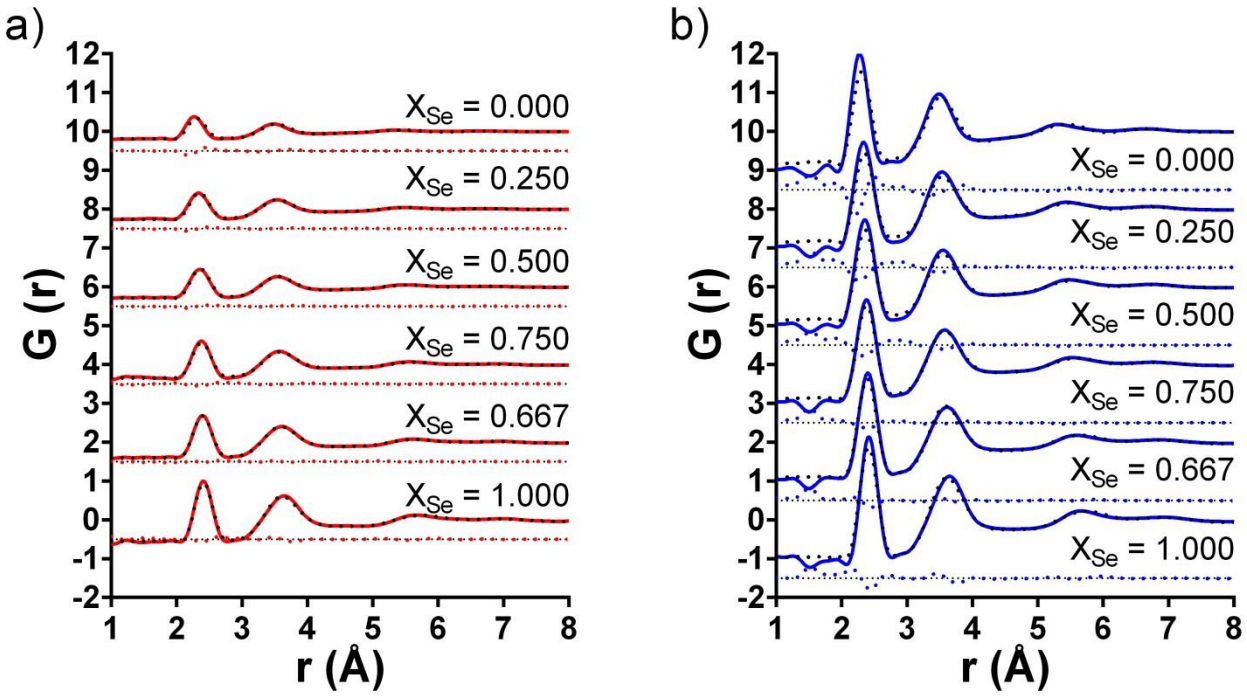

Figure S5: Experimental a) neutron (solid red) and b) X-ray (solid blue) radial distribution functions, G(r), plotted with those produced from the MC-EPSR simulations with Lone Pairs (black dotted lines) for each of the As-S-Se glasses studied. The residuals are shown using coloured dotted lines and these data are shifted to aid clarity.

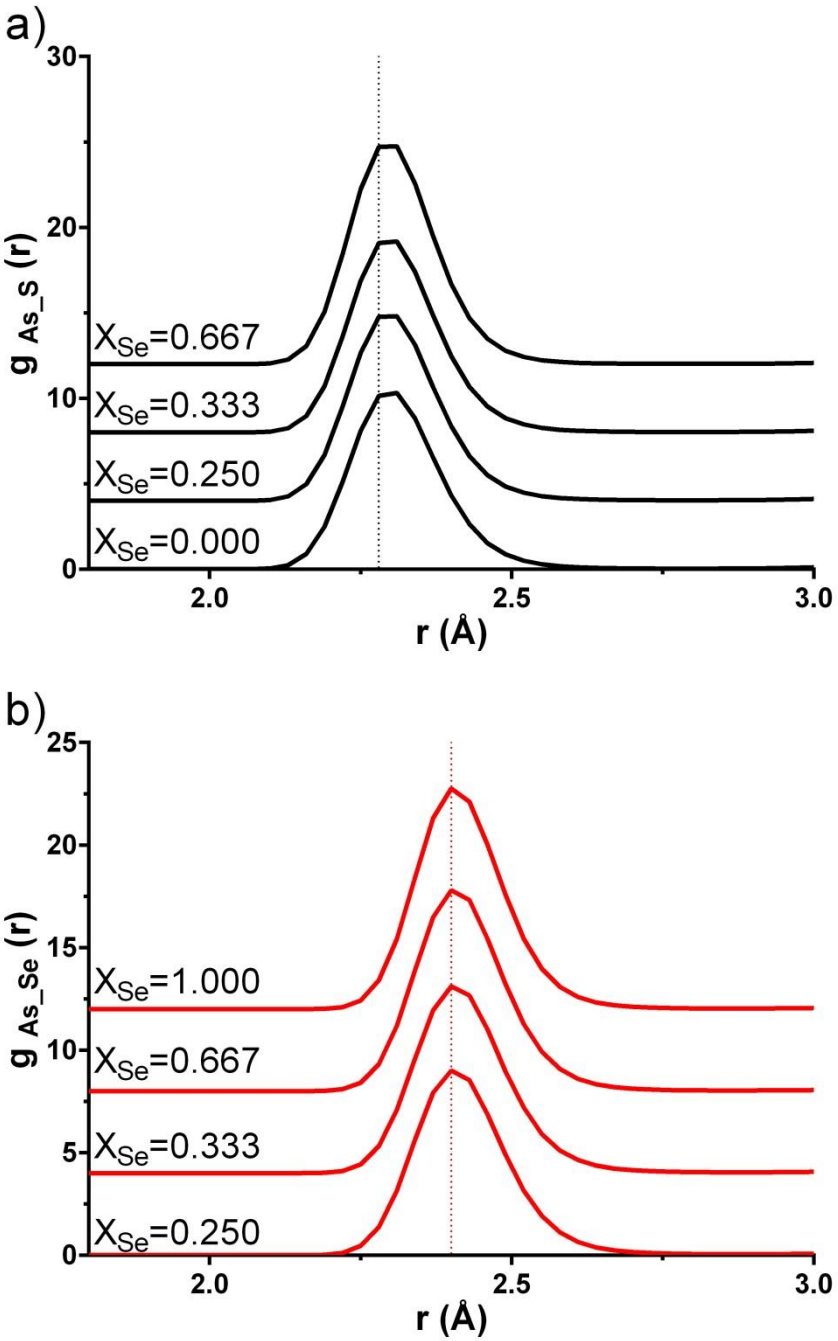

Figure S6: Partial radial distribution functions, $g_{As\text{-}Ch}(r)$, for a) arsenic-sulphur (black) and b) arsenic-selenium (red) taken from the MC-EPSR simulations with Lone Pairs for each of the As-S-Se glasses studied. The dotted lines indicate the expected position of the peak as calculated using bond valence.

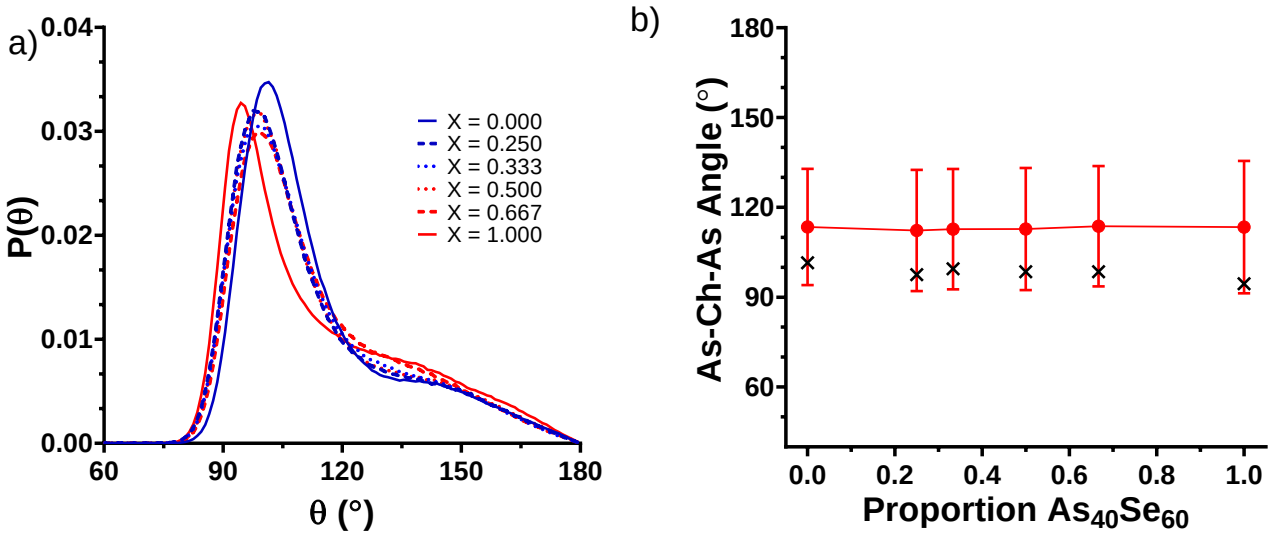

Figure S7. a) The angular distribution of arsenic atoms around each chalcogen atom (As-Ch-As) taken from the Lone-Pair configurations for MC-EPSR. b) The mean (black crosses) and modal (red circles) averages and standard deviations for bond angles.

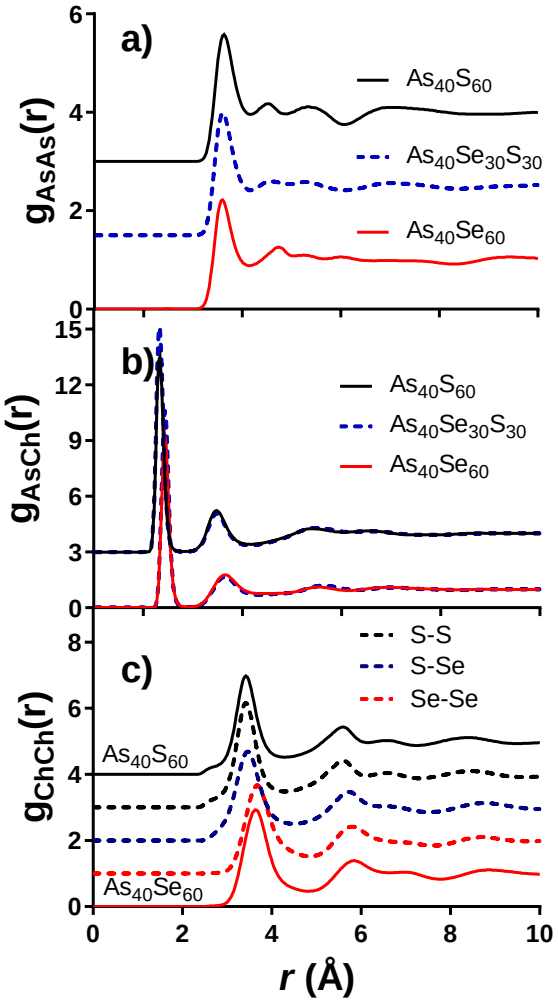

Figure S8: The partial correlation functions generated using Lone-Pair MC-EPSR for $As_{40}S_{60}$, $As_{40}S_{30}Se_{30}$ and $As_{40}Se_{60}$. These include a) the As-As partial correlation functions, b) The As-Ch correlation functions, where the As-S and As-Se partials simulated for $As_{40}S_{30}Se_{30}$ (blue dashed) and superimposed on those for $As_{40}S_{60}$ (black) and $As_{40}Se_{60}$ (red), and c) the Ch-Ch partials where the Ch-Ch partials for $As_{40}S_{30}Se_{30}$ are shown as dashed lines.

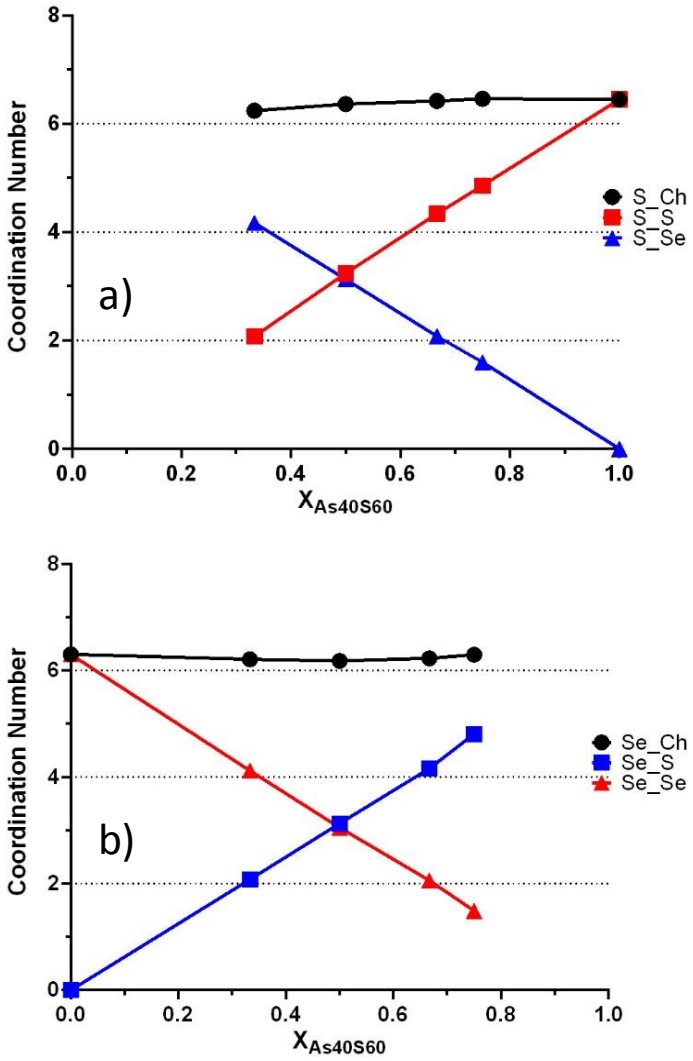

Figure S9: The chalcogen-chalcogen coordination numbers, n_{ChCh}, for each glass composition calculated using the Lone Pair MC-EPSR models over a distance range 0-4 Å. a) gives the total number of chalcogen neighbours around a sulphur atom and b) gives the total number of chalcogen neighbours around a selenium atom