

Structure and dynamics in aqueous mixtures of glycerol: insights from molecular dynamics simulations

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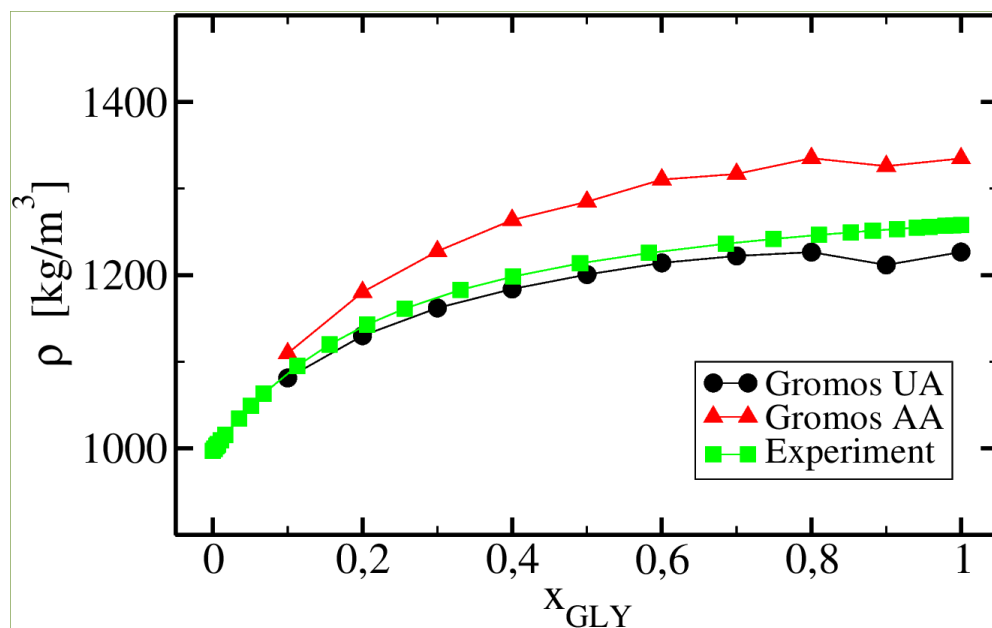


Figure S1. Density ρ vs. glycerol concentration x_{GLY} in UA glycerol-water (black dots) and AA glycerol-water (red triangles). Uncertainty of the data is up to 5 kg/m^3 (for mixtures) and about 20 kg/m^3 for pure glycerol. Lines are just guidelines for the eye. Experimental results are from Ref. 46 in the main manuscript.

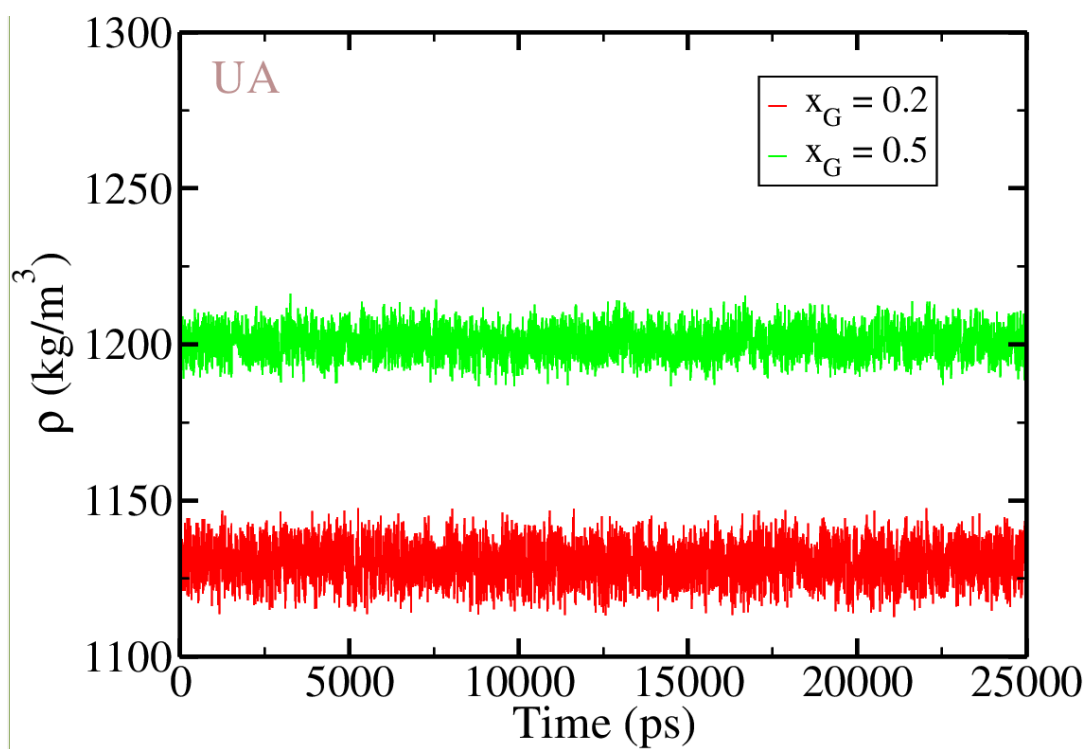


Figure S2. Density ρ versus time t for two selected concentrations $x_G=0.2$ (red line) and 0.5 (green line).

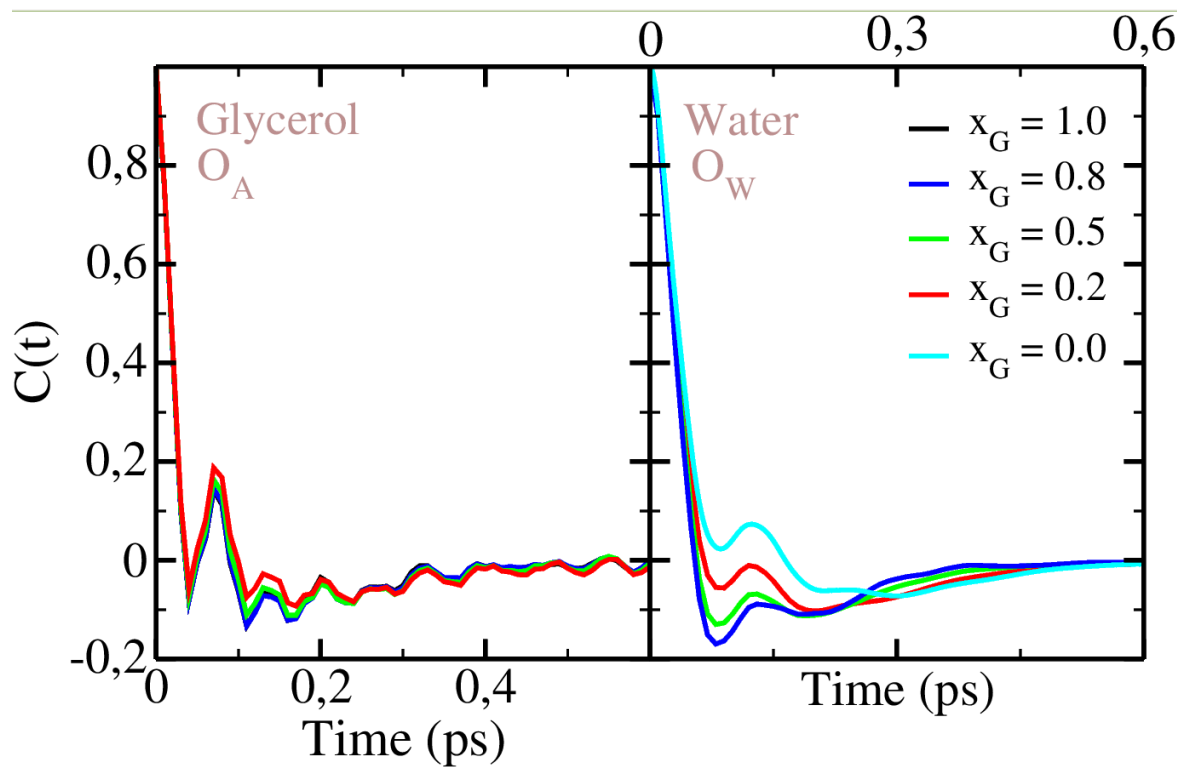


Figure S3. Velocity autocorrelation function $C_v(t)$ for O in glycerol AA model (left panel) and O in water (right panel). Color convention: $x_G=1.0$ (black), $x_G=0.8$ (blue), $x_G=0.5$ (green), $x_G=0.2$ (red), $x_G=0.0$ (cyan).

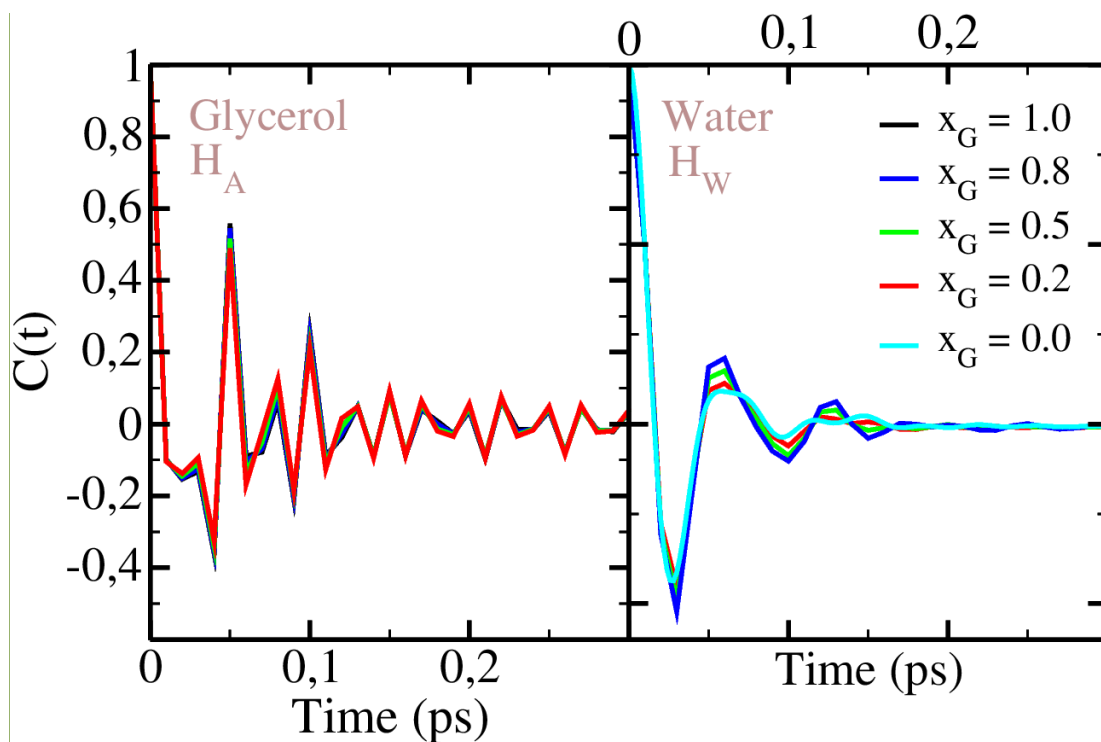


Figure S4. Velocity autocorrelation function $C_v(t)$ for H in glycerol UA model (left panel) and H in water (right panel). Color convention: $x_G=1.0$ (black), $x_G=0.8$ (blue), $x_G=0.5$ (green), $x_G=0.2$ (red), $x_G=0.0$ (cyan).

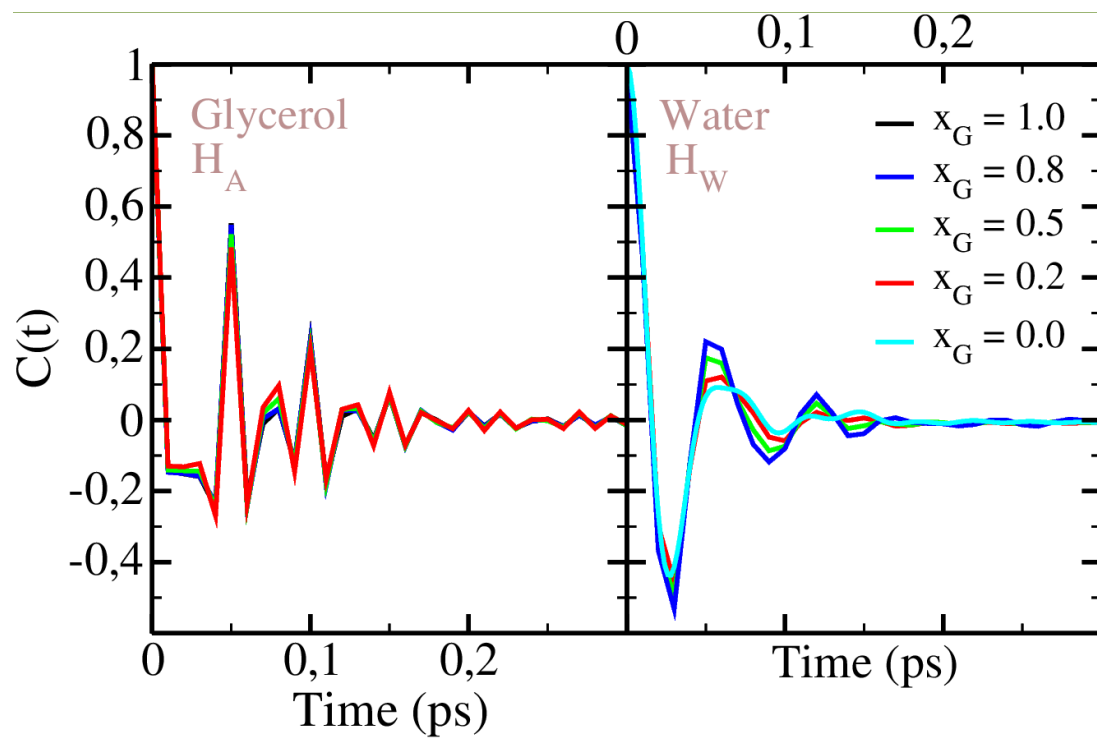


Figure S5. Velocity autocorrelation function $C_v(t)$ for H in glycerol AA model (left panel) and H in water (right panel). Color convention: $x_G=1.0$ (black), $x_G=0.8$ (blue), $x_G=0.5$ (green), $x_G=0.2$ (red), $x_G=0.0$ (cyan).