The Effect of Cosolvent Concentration on Mixing in Nanoconfined Solutions

Rita Okumu ('14)[‡], Amanda Fadling[‡], Randall Ferguson[‡],

Valeria Molinero[*] and Tricia D. Shepherd[‡]

[‡]Westminster College, Salt Lake City, UT 84105

[*]Department of Chemistry, University of Utah, Salt Lake City, UT 84112

We use Molecular Dynamics simulations to investigate the concentration dependence of mixing for a confined aqueous system. Our set-up is comprised a solution enclosed within a nanopore made of fixed water molecules.[1] We include a reservoir containing water and solute at one end of three different systems: one with water only, a second with water confined in a pore, and a third similar to the second system but with polymers grafted onto the walls. For each system, the amount of cosolvent is varied to achieve a specific concentration. The mixing of the cosolvent within the reservoir and then throughout the remaining system is analyzed as a function of time. Results from these simulations should provide further insight into relatively new disciplines, such as cellular biophysics, which rely heavily on microfluidics.

References

1 V. Molinero and E.B. Moore, J. Phys. Chem. B, 2009, 113, 4008