

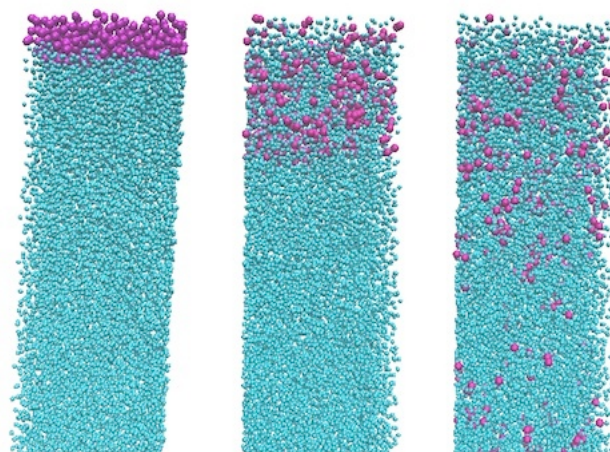
The Effect of Cosolvent Polarity on Mixing in Nanoconfined Solutions

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Our research explores construction of a model that simulates the mixing of water and solute in a nanopore. Water is described by the course-grained model, mW, which represents each water molecule as a single particle.¹ An idealized “pore” is modeled as a group of water molecules restrained from diffusing into the surrounding solvent.² In order to better understand cosolvent dynamics within a nanopore, solvent interactions are considered in a stepwise manner: first as part of an isolated reservoir, then as part of an expanded cell the size of the pore, and finally as part of the full pore model. The force field used for our course-grained simulation is the Stillinger-Weber (SW) potential.¹ Solvent properties can be manipulated by selecting different values for epsilon (ϵ) and sigma (σ) parameters. The parameter ϵ corresponds to depth of the potential describing the attractive interactions between solvent particles, thus larger ϵ values correspond to a more miscible solute. The parameter sigma (σ) refers to repulsion between solvent particles. In effect, these properties can be used to distinguish between hydrophobic/philic cosolvents. Analysis of density profiles and radial distribution functions are used to compare the extent of mixing for each system.



References

- 1 V. Molinero and E.B. Moore, *J. Phys. Chem. B*, 2009, **113**, 4008
- 2 E. Llave, V. Molinero and D.A. Scherlis, *J. of Chemical Physics*, 2010, **133**, 034513