Investigating the hydration of solutes with both hydrophobic and hydrophilic character

Jessie Eiting[‡], Tricia D. Shepherd[‡], Valeria Molinero[*]
[‡]Westminster College, Salt Lake City, UT 84105
[*]Department of Chemistry, University of Utah, Salt Lake City, UT 84112

Molecular dynamics simulations performed by LAMMPS are used to study the hydration of a diatomic system where one particle is hydrophilic and the other is hydrophobic. By varying the bond length between the two particles, it is possible to see hydration trends as it transitions from more hydrophilic (short bond lengths) to more hydrophobic (larger bond lengths). As the bond length increases, disruption of the hydration shell is observed as the molecule becomes more polar. By introducing various bond lengths of the polar molecule into an environment with a water-vacuum interface, it is possible to see the patterns in the preferred orientation and position of the molecule with respect to the interface. These findings will help research in clathrates by giving a greater understanding of the interactions between water and similar molecules in a quasi-liquid interface. With a better grasp of the interaction mechanics, the growth and properties of clathrates can be better understood.