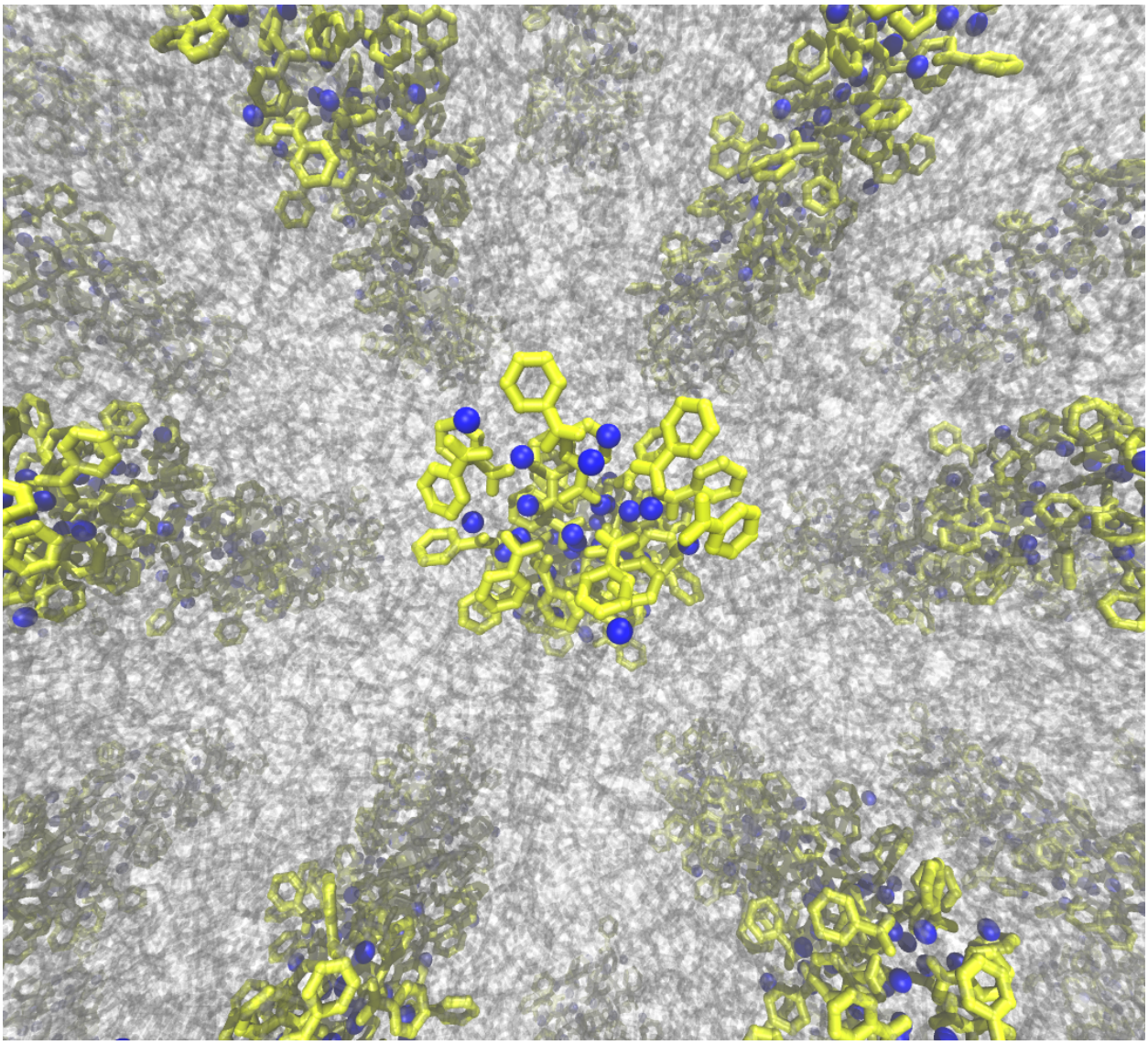

We studied the atomistic structure of a lyotropic liquid crystal (LLC) membrane using molecular dynamics simulations run for hundreds of nanoseconds enabled by Bridges GPU nodes. We learned that the membrane pores (represented by blue sodium ions and yellow LLC monomer head groups above) are dense with a gradual transition from hydrophilic to hydrophobic character as distance from the pore center increases. We will use our model, which has been validated with experimental studies, in order to characterize transport of small molecules inside the nanopores so we can learn how to design new LLC membranes for solute-specific separations.