

Molecular Dynamics of glycerol under nanoconfinement

Dr Alessandro Patti, University of Manchester, UK

We have performed Molecular Dynamics simulations of glycerol in γ -Al₂O₃ nanopores to shed light on controversial observations reported in the literature regarding the dynamics of viscous fluids under confinement. We found that the presence of the solid/liquid interface and the liquid/gas interface in partially saturated pores dramatically determine the disruption of the hydrogen bond network of glycerol. Despite the reduction of hydrogen bonds between glycerol molecules far from the solid surface, glycerol molecules near the solid surface can establish hydrogen bonds with the hydroxyl groups of γ -Al₂O₃ that significantly slow-down the dynamics of the confined fluid compared to the bulk liquid. On the other hand, the disruption of the hydrogen bond network caused by the liquid/gas interface in unsaturated pores reduces significantly the number of hydrogen bonds between glycerol molecules and results in a faster dynamics than in the bulk liquid. Our simulation results suggest that the discrepancies reported in the literature are a consequence of measurements carried out under different pore saturation conditions.