ENHANCED DYNAMICS OF GLYCEROL IN GAMMA-ALUMINA NANOPORES

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Equilibrium and transport properties of fluids are deeply affected under 2D or 3D confinement [1]. Knowledge of molecular level properties of confined systems is especially relevant in a wide spectrum of technological applications, including catalysis, oil recovery and membrane separations [2]. Of special interest is the case of viscous glass-forming liquids in mesoporous materials, where a deeper understanding of the physics of the fluid under confinement, based on relationships between structure and mobility, is required in order to fully understand thermodynamic and kinetic properties [3]. Particle-based simulations can provide a detailed insight into this multifaceted problem [4], which is dramatically determined by the complex nature of inter-molecular interactions. In this work, we present results from classical Molecular Dynamics (MD) simulations of condensed interfacial-Glycerol on Gamma-Alumina. Model systems of slit-shaped pores at different degree of saturation are studied. The heterogeneity imposed by the presence of the solid surface is analysed in terms of the dynamic and structural properties of the liquid in the proximity of the interface and sufficiently far from it. In particular, spatial ordering of Glycerol into quasi-discrete molecular layers is observed and the confinement is also seen to influence the relaxation dynamics as a result of the slowing down of the average molecular motion (translational and rotational) at the solid-liquid interface. In the case of slit-shaped pore geometries at full saturation, this results in an overall decrease of the molecular self-diffusion when compared to the unperturbed bulk fluid at the same density. Interestingly, an accelerated dynamics is detected for the outermost layers of glycerol molecules in the unsaturated pores. Such a behaviour could explain the enhanced self-diffusion of Glycerol on Gamma-Alumina that has been reported in recent experimental observations [5].

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