Properties of a confined molecular glass-forming liquid

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Résumé en anglais	We use molecular dynamics (MD) simulations to investigate the modification of the dynamic and static properties of liquid toluene when confined in cylindrical mesopores a few molecular diameters across. Due to the strong influence of the substrate on the dynamics of the confined liquid, we choose a procedure where no additional thermal interactions between the wall and the liquid are taken into account. We observe the characteristic oscillations of molecular density profiles (layering) when temperature and pore size are changed. Mean square displacements and intermediate incoherent scattering functions of the centre of mass of the molecules are calculated as functions of different distances from the wall along the principal axis of the pore z and along the perpendicular x- and y-directions. At 200 K the relaxations of the two correlation functions slow down by one order of magnitude as compared to the bulk, with a slightly more pronounced slowing down in the x-direction. This slowing down increases strongly when the wall is approached. However, we do not observe any layer-specific dependence of the dynamics, but instead a continuous change. When the molecules are arrested near the wall in the time window (1 ns) of the simulations, we find hopping processes.
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