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Mobility of water and selected atoms in bilayer DMPC membranes[1] F.Y. HANSEN, Technical University of Denmark, H. TAUB, M. BAI, A. MISKOWIEC, University of Missouri-Columbia — Molecular dynamics simulations have been used to determine the mobility of water molecules as a function of their positions in a fully hydrated free standing DMPC membrane at 303 K. In a 10 Å thick water layer with bulk density just outside the membrane, the mobility of the water molecules is reduced by about a factor of two relative to bulk. For water molecules penetrating deeper into the membrane there is an increasing reduction in the mobility with up to two orders of magnitude for those deepest into the membrane. A comparison with the mobility of selected atoms in the lipid molecules shows that about 5 water molecules/lipid molecule move on the same time scale as the lipid molecules and may therefore be considered to be so tightly bound to them that they essentially follow their motion. The simulation results are quantitatively compared with quasielastic neutron scattering results on single-supported bilayer DMPC membranes.

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