Lipid bilayer membranes under shear flow from molecular simulations

Alexandru Botan, Laurent Joly, and Claire Loison

[1] *Institut Lumière Matière, Université Lyon 1,*
69622 Villeurbanne, France – claire.loison@univ-lyon1.fr

Abstract

According to the World Health Organization every tenth person in the world suffers from joint pain associated with arthritis. In this disease there is a disturbance in regeneration of tissues which prevent direct contact of bones making up the joint. Particularly, the deficiency of synovial fluid causes stiffness and pain as well as destruction of cartilage. The point is that synovial fluid reduces friction between the articular cartilage of synovial joints during movement to extremely low values (0.005-0.04), that is much lower than values attained using any synthetic bearing materials in equivalent situations. To explain these values, a fluid film mechanism, where the two sliding surfaces are separated by a thin hydrophobic layer of the lipid bilayers (a component of synovial fluid), has been proposed. The molecular structure of the lipids, their organization, hydration level are called the major factors responsible for such low friction[1]. To quantify their influence we model lipid bilayers under a shear using non-equilibrium molecular dynamics simulations (NEMD). In this approach, water is confined between two lipid bilayers, and the shear flow is induced by moving the top and bottom membranes in opposite directions at constant velocity. Molecular configurations are then used to provide insight into the interactions of lipids with water. The results are compared with experimental data.

[1] K.Falk, N. Fillot, A.-M. Sfarghiu, Y. Berthier and C.Loison *Phys.Chem.Chem.Phys.*, 2014,16, 2154-2166.