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Diffusion in a hard-disk fluid with immobile particles: Molecular transport in the plasma membrane

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With respect to lateral diffusion of molecules, plasma membrane of living cells can be thought as a two-dimensional fluid that is coupled to the underlying cytoskeleton. As the dynamics of cytoskeletal structures are often much slower than that of lateral diffusion, membrane proteins can become immobilized by anchoring to the cytoskeleton via direct or indirect binding. Motivated by single particle tracking observations showing that even lipid molecules are strongly affected by the membrane-cytoskeleton coupling [1], we study the effects of immobile particles on lateral diffusion. By considering a two-dimensional hard-disk fluid, which is relevant when repulsive interactions are dominant, we explicitly account for fluid dynamical interaction between particles. We perform event driven molecular dynamics and Brownian dynamics simulations of a collection of hard-disks. We focus on fluids composed of uniform disks as well as binary mixtures. In the case of uniform disks, we envisage mobile particles as lipids and immobile particles as proteins anchored to the membrane skeleton. In binary mixtures, proteins and lipids are represented by disks of different radius and mass (see Fig. 1).

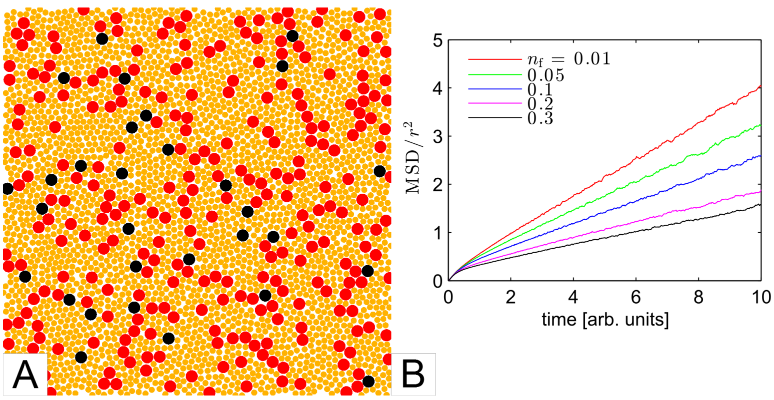

Figure 1: In A, a snapshot from the event driven molecular dynamics simulation is displayed, where red (larger) and orange (smaller) disks represent proteins and lipids, respectively, and the disks in black are immobile. The total packing fraction, that is the area covered by all disks, is equal to 0.75. In B, the mean squared displacement of larger disks (averaged over 100 particles), normalized by the square of the radius of smaller disks, r^2, is plotted as a function of time for different values of the fraction of fixed disks (denoted by n_f).

In the regime where the mixture is in the liquid state with a packing fraction of 0.5–0.75, we find that the particles are diffusive at long times, and the diffusion coefficient is very sensitive to the fraction of immobile particles. We study the effects of random and correlated distributions of immobile particles on diffusivity, as well as the effects of particles that are only temporarily immobilized. In previous studies [2, 3], it has been shown that fluid dynamical interactions can lead to a significant drop in diffusion coefficients in membranes containing immobile inclusions. However, the membrane was treated like a continuous fluid, which is only valid at length scales much larger than that of a lipid molecule. In this respect, we believe that our study fills an important gap between the molecular and macroscopic scales in describing the effects of fluid dynamical forces on lateral diffusion in the presence of immobile particles.

References

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