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Diffusion in a discrete two-dimensional 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 is often much slower than that of lateral diffusion, membrane molecules can become immobilized by anchoring to the cytoskeleton via direct or indirect binding. Motivated by these observations, we study the effects of immobile particles on lateral diffusion, by modeling the membrane as a two-dimensional hard-disk fluid. We perform event driven molecular dynamics and Brownian dynamics simulations of a binary mixture of hard-disks, where proteins and lipids are represented by disks of different radius and mass. In the parameter regime where the mixture is in the liquid state with a packing fraction of more than 0.5, we find that the particle motion is 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. Previous studies [1,2] that accounted for fluid dynamical interactions treated the membrane as 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.

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[2] N Oppenheimer and H Diamant. In-plane dynamics of membranes with immobile inclusions. Phys. Rev. Lett., 107(25):258102 (2011).