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Contributed talk 7 - Influence of shape and interaction anisotropy on short-time protein diffusion

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In a dense and crowded environment such as the cell, an individual protein feels the presence of surrounding proteins. It is thus expected that direct and hydrodynamic interactions strongly affect the diffusion of proteins. Examples are suspensions of eye lens proteins, where a dramatic slow down of the local short-time diffusion of γB-crystallin and a dynamical arrest is observed experimentally under crowded conditions. Here, we demonstrate that an application of colloid models, together with appropriate theoretical and simulation tools that allow to incorporate direct and hydrodynamic interactions, provides detailed insight into the dynamics of protein solutions. The hybrid simulation approach combines the multiparticle collision dynamics (MPC) method for the fluid with molecular dynamics simulations (MD) for the globular proteins. We present results for the short-time diffusion of different model proteins, where their dynamics are analyzed together with structural properties. The effect of shape anisotropy as well as weak attractive patches between colloids are discussed. In particular, we highlight the dramatic effect of weak interaction anisotropy known to exist between many globular proteins on the short-time diffusion under crowded conditions. This study is of great interest in applications such as formulations as well as for the fundamental understanding of soft matter in general and crowding effects in living cells in particular.

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