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Multiscale Approach for Hydrated Systems: From Nano-Materials to Perspectives for Brain Cancer Treatments

Giancarlo Franzese
Universitat of Barcelona, Spain
Institute of Nano-science and Nanotechnology (IN2UB)

The Blood-Brain-Barrier (BBB) is the tight membrane that protects our brain and represents the major hindrance to the use of chemotherapeutic agents for brain tumors.

Recently it has been showed by *in vitro* and *in vivo* studies that the adsorption of apolipoprotein E4 (ApoE4) on lipid nanoparticles (NPs) produces a protein corona that enhances the BBB-crossing, improving brain NP accumulation 3-fold compared to undecorated particles. Therefore, it is possible to increase the ability to cross the BBB for engineered NPs carrying a loose layer of proteins. Nevertheless, the NP-protein corona composition—and, as a consequence, the cellular biological response to the NP—change over time as a consequence of the competition among the plasma proteins once the NP is in the blood stream, as we showed.

In collaboration with experimental groups, we develop a multiscale approach for the study of bio-membranes, proteins, NPs and nanomaterials in aqueous solution oriented to applications to the BBB crossing for oncological treatments. We model the kinetics of NP interaction with proteins,of proteins with water, and of water with membranes and nanomaterials, with the aim of finding how to optimize the NP-protein corona formation to cross the BBB.

We will describe our recent results by all-atom simulations and coarse-grained models, e.g. showing that the water-membrane interface has a structural effect at ambient conditions that propagates further than the often-invoked 1 nm length scale and that the translational and rotational dynamics of water molecules is strongly determined by their local distance to the membrane so that we can identify the existence of an interface between the first hydration shell, partially made of hydration water bound to the membrane, and the next shells entirely made of unbound hydration water. These results could drastically affect the kinetics of the protein-corona, determining the fate of NPs during the BBB crossing.

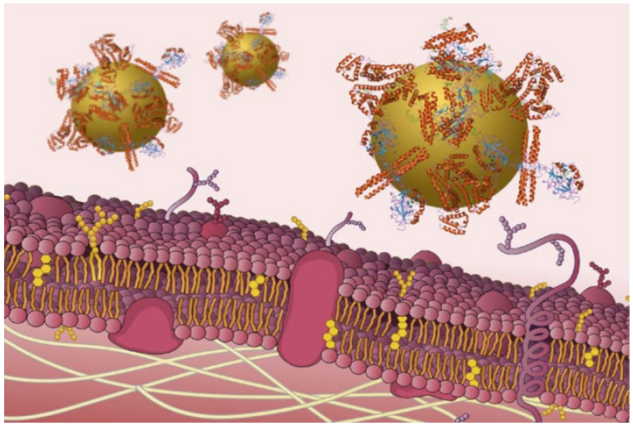

Figure: Cartoon of NP-Protein corona complexes near a cellular membrane.