Molecular modelling of the protein corona for nanoparticles

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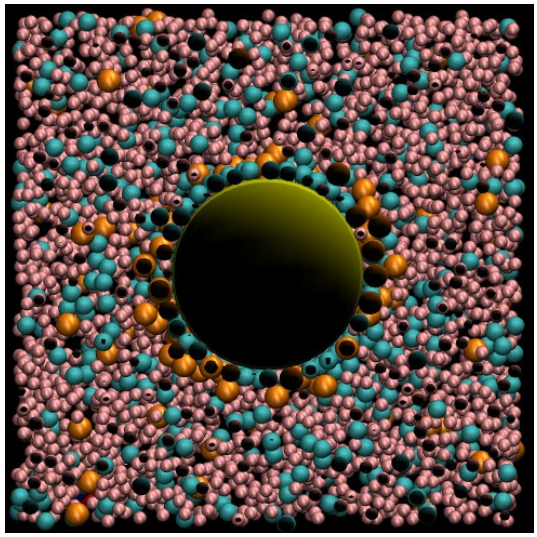
Abstract

Nanoparticles (NP) in the extracellular matrix are immediately coated by layers of biomolecules forming a "protein corona". This protein corona gives to the NPs a "biological identity" that regulates the NP-cell interaction. Therefore, the cell uptake of the NPs is strongly affected by the protein corona. For this reason learning to predict the biological identities of NPs based on a partial experimental knowledge is essential to foresee *a priori* the safety implications of a NP for human health and, more in general, the environment.

To this goal we propose a multiscale approach that allows us to predict the protein corona composition based on a partial experimental knowledge. The approach, both theoretical and computational, includes protein-protein [1] and protein-NP interactions, accounting for the physico-chemical properties (electrostatic and Van der Waals interactions) and the size of the NPs as in the DLVO theory for colloids.

We study, by numerical simulations, the competitive adsorption of proteins on a single NP suspended in blood plasma as a function of contact time and plasma concentration. We consider the case of silica NPs in a "simplified" blood plasma made of three competing proteins: Human Serum Albumin, Apolipoprotein A1 and Fibrinogen. These proteins are of particular interest because they are present in high concentrations in plasma, or because they are the most abundant in the corona of silica NPs [2]. Our results are compared with experiments made under the same conditions showing that the approach has a predictive power [3].



References

[1] P. Vilaseca, K.A. Dawson, G. Franzese *Understanding and modulating the competitive surface-adsorption of proteins*, Soft Matter, **9**, 6978 (2013)

[2] S. Milani, O. Vilanova, K. A. Dawson, G. Franzese and J. Rädler, *The Protein Corona in a Three Component Model Plasma* (in preparation)

[3] O. Vilanova, S. Milani, K. A. Dawson, J. Rädler and G. Franzese, *Theoretical and Numerical Predictions Compared to Experiments for Silica Nanoparticles in a Three Component Model Plasma* (in preparation)