Mass transport phenomena at solid-liquid nanoscale interface in biomedical applications

Annalisa Cardellini[*], Matteo Fasano[†], Eliodoro Chiavazzo[†] and Pietro Asinari[†]

[*†]Multi-scale-Modeling-Laboratory, Dipartimento di Energia (DENERG),
Politecnico di Torino,
Corso Duca degli Abruzzi 24, 10129 Torino, Italy
e-mail: annalisa.cardellini@polito.it, web site: http://www.polito.it/small

ABSTRACT

Coupling nanoscience with biomedical application has shown promising results in the recent years: for example, engineered nanoporous material are often used for targeted drug delivery, whereas specific nanoparticles show theranostic potential [1]. For this reason, the understanding of heat and mass transfer phenomena at solid-liquid nanoscale interface plays a crucial role for introducing novel and more rationally designed theranostic particles or drug with tailored features. For instance, the water transport properties in the proximity of contrast agents are critical for Magnetic Resonance Imaging: a reduction of water diffusivity, in fact, may imply a significant improvement of the diagnostic performances [2].

In a previous work, the transport behavior of water molecules in nanoconfined conditions has been investigated. By means of equilibrium Molecular Dynamics (MD), water self-diffusion coefficients have been evaluated; then, a relevant dimensionless variable ϑ (i.e. the ratio between nanoconfined and total water volumes) has been suggested for water self-diffusivity in a large variety of configurations. A scaling behavior for transport properties in nanoconfined geometries has been consequently demonstrated [3].

Then, more detailed analyses have been focused on water self-diffusion close to biomolecules such as proteins and amino acids. Moving from proteins to their building blocks (i.e. amino acids), a similarity in water behavior was initially expected.

The MD simulations results have been used to underline the main differences between the two cases: proteins on one hand and amino acids on the other hand. Specifically, the comparison has been performed by considering their characteristic length of nanoconfinement δ. The latter is defined as the distance between a water molecule and the solid surface where the attractive nonbonded interaction of the solid prevails on the kinetic energy of the liquid.

The analysis of several proteins and all amino acids has shown a consistent mismatch: the almost constant values of δ among different proteins ($\delta_{pro} \cong 0.3\ nm$) was significantly larger than the typical amino acids characteristic lengths ($\delta_{aa} \cong 0.19\ nm$).

Results indicate that the reduction of water mobility in the proximity of nanoscale interfaces does not rely only on the local physical and chemical properties of the biomolecules surface, but the effects of size and potentials overlap should be also taken into account. Moreover the variety of amino acids configurations in proteins does not allow a trivial prediction of δ_{pro} once δ_{aa} of the constituents are known.

REFERENCES

[1] Gizzatov a. et al., Hierarchically Structured Magnetic Nanoconstructs with Enhanced Relaxivity and Cooperative Tumor Accumulation, Adv Funct Mat 24, 4584 (2014)

[2] Ananta J., Biana Godin, Richa Sethi, Loick Moriggi, Xuewu Liu, Rita E. Serda, Ramkumar Krishnamurthy, Raja Muthupillai, Robert D. Bolskar, Lothar Helm, Mauro Ferrari, Lon J. Wilson & Paolo Decuzzi, Geometrical confinement of gadolinium-based contrast agents in nanoporous particles enhances T1 contrast, Nat. Nanotech. 5, 815 (2010)

[3] Chiavazzo E., Fasano M., Asinari P. and Decuzzi P., Scaling Behavior for the Water Transport in Nanoconfined Geometries, Nature Communications 5, 4565 (2014)