A Nano-scale view of Protein hydration Water at Low Temperature

María Carmen Morón[1,2].
[1] Instituto de Nanociencia y Materiales de Aragón, CSIC-Universidad de Zaragoza.
[2]Departamento de Física de la Materia Condensada, Facultad de Ciencias, Universidad de Zaragoza.

Water affects every aspect of our lives. It constitutes a transversal and sustainable subject of research. With a ubiquitous character, biomolecules like nucleic acids or proteins are immersed in it. However water should not be regarded as just a solvent. The shell of water molecules in close interaction with a biomolecule surface is called *biological water*. That peculiar water is essential to biomolecule structure, dynamics and function.

In this communication, the dynamics of the hydration layer of the protein Barstar is followed at room and low temperature (300-243 K), using all-atom molecular dynamics simulations, and correlated with that of isolated water:

1. *A stretched exponential function* $exp[-(t/\tau)^{\beta}]$ describes the room and low temperature relaxation of residence times of water molecules in the protein hydration layer. The value of the stretched exponent $\beta = 0.48 \pm 0.01$, clearly departing from 1, validates the presence of remarkable temporal disorder in the system and *multiple decay time scales*. The existence of those multiple scales has been also detected at *nanoscopic level*. On the other hand as temperature goes down the relaxation time τ increases, exhibiting a divergence at a *transition temperature* $T_L = 226 \pm 4$ K.

2. A power law temporal distribution, $t_r^{-\alpha}$ (t_r stand for the residence time of water molecules at the protein surface, $\alpha = 0.63 \pm 0.07$), shows the *scale-free character of the dynamics* in the case of protein hydration water (see Fig. 1). Surprisingly, an equivalent scale-free dynamics has been also detected for isolated water ($\alpha = 0.58 \pm 0.09$). Nevertheless the *maximum residence time in the case of protein hydration water is two orders of magnitude larger than for isolated water*. Then the biomolecule but also the solvent, are responsible for the heterogeneous dynamics protein hydration water exhibits. *Biological water notices both 'scenarios' and, since the three entities must coexist at the same time, tries to accommodate them.*

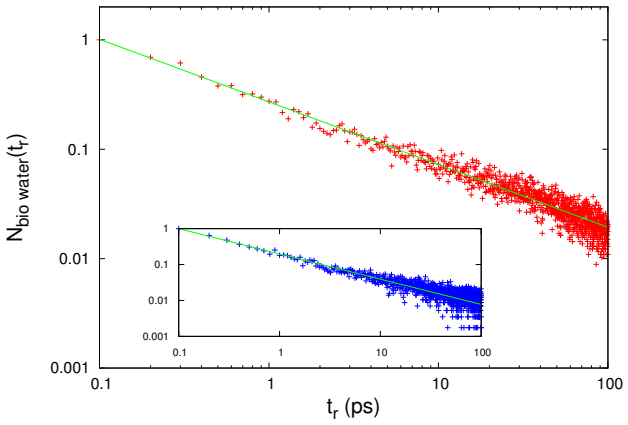

Fig. 1. Scale-free dynamics: normalized number of water molecules as a function of the time they spend within a cut-off of 0.40 nm from the protein surface at 288 K (inset at 243 K).

3. *Comparison with experimental data is presented along the work. Experimental results are quantitatively reproduced.*

[1] M.C. Morón, Journal of Molecular Liquids **272** 902-911 (2018).