Slow dynamics and local structure of water at interfaces

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Recent Molecular dynamics simulation results of the behavior of water at interfaces are discussed for three systems: water in the proximity of a protein, water and trehalose in proximity of a protein, the Lysozyme, and water and premelting-layer/ice in the proximity of an ice nucleating particle (INP), the K-Feldspar, present in the atmosphere. Translational dynamics of the hydration water of a Lysozyme protein upon cooling is studied through the self van Hove function and the mean square displacement [1]. In the deep supercooled region it shows two different temperature activated relaxation mechanisms. The low-temperature hopping regime has a time scale of tenths of nanoseconds and a length scale on the order of 2–3 water shells and it is also present in bulk water. The second hopping regime is active at high temperatures, on the nanoseconds time scale and over distances of nanometers. This regime is connected to water displacements driven by the protein motion and it is observed very clearly at high temperatures and for temperatures higher than the protein dynamical transition. Modification of dynamics in presence of trehalose is discussed [3]. A detailed local structural analysis assessing the difference between the hydration water influenced by the protein and bulk water in terms of high density and low density distribution in local structures is also shown and discussed [2]. Finally results on the local structure of supercooled water and of the premelting layer and ice in vicinity of K-Feldspar with the aim to study the affinity of this INP with ice are shown [4]. This latter system is studied at two different pressures.

REFERENCES

[1] L. Tenuzzo, G. Camisasca and P. Gallo Molecules, 25 (2020) 4570
[2] G. Camisasca, L. Tenuzzo and P. Gallo, in preparation (2022)
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[4] B.V. Ramirez, L. Lupi and P. Gallo, submitted (2022)

FIGURES

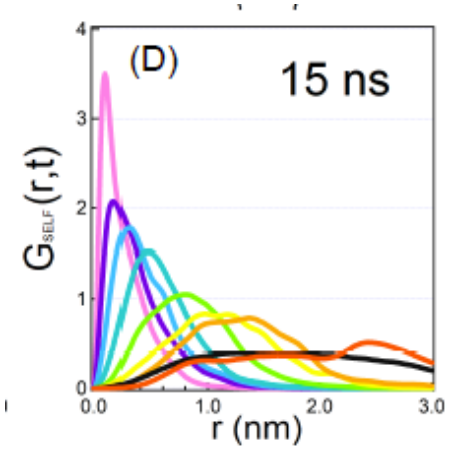

Figure 1: Long time hopping phenomena in the Van Hove Self Correlation Function of Hydration Water in the proximity of lysozyme. The different curves, calculated for time t=15ns, span from T=200 K (Pink curve) to T=300 K.