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S E M I N A I R E

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« Water thermodynamics and its effects on biological interfaces »

All-atom simulations of large-size systems including proteins and explicit water come at a great computational cost. To overcome this problem, coarse-grained models aim to represent the system in a simplified manner but keeping the essential properties that are relevant for its behavior. In this seminar, we extend to bulk a coarse-grained model, with many-body interactions, originally introduced by Franzese and Stanley (FS) for water monolayers [1, 2], that is analytically tractable and can be equilibrated by efficient cluster Monte Carlo for large systems (10^7 molecules) at extremely low temperatures (deep supercooling) in a wide range of pressures (both negative and positive) [2].

In its original formulation, the FS model reproduces qualitatively, the experimental water phase diagram, clarifying the physical mechanisms of the different scenarios proposed for the thermodynamic and dynamic anomalies of water, including the liquid-liquid phase transition and its Widom line. Also, it allows interpreting the multiple dynamic crossovers observed experimentally in protein hydration water, and more recently in melted water layers, at variance with atomistic models. Its application to hydrated proteins rationalizes the contribution of water to pressure and cold denaturation, generalizes the protein design to any thermodynamic condition, and clarifies the condition for protein aggregation [3].

Our results for the bulk FS model compare well with water atomistic simulations and shed light on the microscopic differences between the dynamics in hydration water and bulk water, showing that at lower dimensionality the cooperativity fluctuations decouple from the density fluctuations [4]. The last part of the seminar will be devoted to the application of the bulk FS model to hydrated large protein systems modeled with OPEP at LBT-IBPC [5]. We show that this novel framework is suitable to estimate the solvation free energy landscape of these systems, and discuss its possible application to derive a hydration water driving-force to proteins simulated with OPEP.

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[3] V. Bianco, G. Franzese, and I. Coluzza, ChemPhysChem 21, 377 (2020).
[4] L. E. Coronas, V. Bianco, A. Zantop, and G. Franzese, arXiv:1610.00419 (2016).
[5] O. Languin-Cattöen, E. Laborie, D. O. Yurkova, S. Melchionna, P. Derreumaux, A. V. Belyaev, and F. Sterpone, Polymers 13, 3912 (2021).

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