Multiscale Approach for Water at Bio-Nano Interfaces

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I will present recent simulations and theoretical results about the dynamics and structure of water at bio-interfaces (proteins and bio-membranes) and nano-interfaces (nanoparticles and graphene sheets). By all-atoms simulations I will analyze how hydrophobic and hydrophilic interfaces affect the properties of the vicinal water [1] and we will use the results in a multi scale approach to develop coarse-grained models for water that allow us to extend our investigations to timescales and length-scales that would be unreachable in atomistic simulations. We will consider applications to nano confined ice formation, protein folding and design, protein crystallization, self-assembly of bio-membranes and nanoparticles-protein-corona [2, 3, 4, 5, 6, 7, 8, 9, 10].