Hydration water, ice-like ordering and means to keep dry

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ABSTRACT

In this talk we shall consider the hydration properties of extensive hydrophobic-like surfaces (like graphene and alkane monolayers) and proteins, and we shall also focus on the filling propensity of hydrophobic cavities and carbon nanotubes.
Our results point out to the existence of a few hydration layers that are both better structured and dynamically slower than the bulk. The tendency of such layers to be oriented in a fashion similar to hexagonal ice will also be revealed. Additionally, we shall show cavity filling to depend on the cavity size (around the nanometric range) and on the hydrophobicity of the material, while revealing the dynamical nature of the process with alternation of filled and dry states.
Finally, a few words will be said on water exclusion and dehydration propensity in proteins, where we shall show that the question of "how to keep dry in water?" should be extended towards "how to do it without sacrificing reactivity?", a subject that holds great relevance in protein binding and drug design.