UNIWERSYTET WARSZAWSKI | CeNT CENTRUM NOWYCH TECHNOLOGII

invites to a seminar by

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Biological Water or Rather Water in Biology?

4th of December 2018 at 2 p.m.

Venue: Centre of New Technologies, Banacha 2C,

Lecture Hall 0142 (Ground floor)

Host: Dr. Piotr Setny

Two messages follow from a critical analysis of our results and the existing literature on interfacial water surrounding biological molecules and assemblies, such as proteins, DNA, or fluid phospholipid membranes. The first one, addressed to biologists and biochemists, who tend to focus their attention primarily to the biomolecules, is that water does matter. Moreover, since the interfacial water layer covering the biomolecule has distinct properties from the aqueous bulk it is often not satisfactory to describe the aqueous solvent merely as a structureless continuum with a dielectric constant of bulk water. Such an approach can capture the longer-range dielectric effects of the solvent on the biomolecule, nevertheless, in many cases local interactions between functional groups at the solute surface with adjacent water molecules are important and require atomistic description. The good news is that in most cases one or two layers of explicit “granular” waters around the solute surrounded by a dielectric continuum represent a satisfactory description of the solvent effects.

A potentially more important message is addressed to our community of physical chemists. While water including its interfacial layer, as well as ions and osmolytes, plays a key role in establishing the homeostasis, it is primarily the biomolecule itself which carries the biological function. It is a fact that individual water molecules and ions in binding pockets of enzymes can play an important role. However, there is little direct evidence that collective motions of the hydration layer are decisive for protein function, potentially save for extreme conditions of strong dehydration or cooling (although even there the degree of water involvement in biological functionality is a matter of debate). As physical chemists who naturally tend to understand water better than biomolecules we may sometimes have a tendency to overemphasize the role of the former at the expense of the latter. For this almost psychological reason and, more importantly, due to the scientific reasoning outlined above I would argue that the term biological water should be dropped. It is perfectly justifiable to talk about water in biology and discuss the role of interfacial water around biomolecules with its distinct properties. However, using the term biological water with all its connotations toward a hypothetical state of cellular “vicinal water” carrying biological function might be bringing us dangerously close to the long overcome concept of “vis vitalis”.

[1] Jungwirth, P.: Biological Water or Rather Water in Biology? Journal of Physical Chemistry Letters 6 (2015) 2449.

[2] Pluharova, E.; Laage, D.; Jungwirth, P.: Size and Origins of Long-Range Orientational Water Correlations in Dilute Aqueous Salt Solutions. Journal of Physical Chemistry Letters, 8 (2017) 2031.