LABORATOIRE INTERACTIONS, DYNAMIQUES ET LASERS

LIDYL-UMR 9222
CEA, CNRS, Université Paris-Saclay

SEMINAIRE LIDYL

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Le Vendredi 7 Décembre 2018 à 11h00
- Bâtiment 522 - Salle 138

"*Biomolecular Hydration Shells: Dynamics and Role in Biochemical Function*"

The structure and function of biomolecules are strongly influenced by their hydration shells. Two key challenges are thus first to determine the extent to which the structural and dynamical properties of these shells differ from those of bulk water, and second to elucidate the role played by water in the functioning of biomolecules.

We will first review the recent advances in theory, simulations and experiment that have led to new and detailed insight in the dynamical properties of water molecules in the hydration shells of proteins and DNA. Three central questions will be addressed: what is the size of the hydration shell? To what degree are the shell water dynamics different from bulk water? And what is the molecular origin of the effect induced by the biomolecule on the water dynamics, is it rather due to the shape of the molecule or to the chemical nature of the exposed groups?

We will then consider the influence of water on the function of proteins, and focus on the role of the hydration shell in the catalytic activity of enzymes. Water is usually depicted as a lubricant which facilitates the protein conformational transitions occurring during enzyme catalysis. Through the study of a paradigm enzyme in a water-cosolvent mixture, we will show that this picture is not justified. We will identify the molecular origin of the catalytic activity enhancement by water, and use it to suggest new routes to optimize enzymatic activities in non-aqueous solvents.

Formalités d'entrée :

Visiteur U.E. *: Se faire connaître au moins 48 heures à l'avance pour l'établissement de votre autorisation d'entrée sur le Centre de Saclay.*
Visiteur hors U.E. *: Se faire connaître au moins 4 jours à l'avance pour les formalités d'entrée et se faire accompagner par un agent CEA.*
Sans autorisation, vous ne pourrez entrer sur le Centre de Saclay. Tél. : 33.1.69.08.74 09- Fax : 33. 1.69.08.76.39 - email : caroline.lebe@cea.fr ou veronique.gereczy@cea.fr
Dans TOUS LES CAS, se munir d'une pièce d'identité (passeport et carte d'identité - pas de permis de conduire)