INSTITUT DE PHYSIQUE ET CHIMIE DES MATERIAUX DE STRASBOURG
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SEMINAIRE IPCMS
Vendredi 23 mars 2018
à 10h30 à l'auditorium

Computational studies on protein mechanics

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Proteins are sophisticated molecular machines that have been improved over billions of years during biological evolution. To elucidate mechanical properties of proteins, we perform molecular simulations and structural analysis. My talk consists of two parts.

Mechanical Unfolding of Membrane Proteins: Single-molecule force spectroscopy by atomic force microscopy allows us to get insight into the mechanical unfolding of membrane proteins. We perform coarse-grained simulation of the mechanical unfolding of membrane proteins to study their unfolding mechanism at the molecular level [1,2].

Continuum Mechanical Description of Proteins: Proteins are complex macromolecules and their structures are anisotropic and inhomogeneous in nature. We illustrate the structural/dynamical properties of proteins with atomic stress/strain tensors [3,4,5]. This method has turned out to be useful in describing protein structural changes associated with pressure deformation [3], biomolecular reactions such as photosignal transduction of photoreceptor proteins [4], ligand migration in heme proteins [6], and mechanical allosteric couplings of enzymes [7].

References:

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[6] A. Tomita, T. Sato, K. Ichiyanagi, S. Nozawa, H. Ichikawa, M. Chollet, F. Kawai, SY. Park, T. Tsuduki, T. Yamato, S. Koshihara, and S. Adachi, *Proc. Natl. Acad. Sci. U.S.A.* 106, 2612 (2009).
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