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BioSim Talk #3
23th June 2026 (Tuesday)
3.00 – 4.30 pm
Institute for Protein Research
University of Osaka (Suita Campus)
4th floor Seminar room

Fabrizio Cleri

IEMN (CNRS UMR8520) and Department of Physics, University of Lille, France; Department of Chemical Systems Engineering, The University of Tokyo, Japan

Molecular simulations of nucleosomes: the micromechanics of DNA damage

In a series of recent works [1-4], we explored by means of molecular dynamics simulations the DNA-protein interactions involving UDG and PARP1 enzymes, in the environment of isolated nucleosomes, di- and tri-nucleosome constructions. Our main focus is on the interplay between DNA plastic deformation and damage/repair mechanisms, and their potential genomic implications. To this end, we developed a protocol to apply external forces to our fully-atomistic systems, and measure mechanical stresses at the molecular level. To study the interaction with repair enzymes, we manually introduced constructs of DNA damage at various sites around the nucleosome, in the form of either a uracil base, targeted by UDG; or clean single- and double-strand breaks, chiefly targeted by PARP1. The ensemble of these results highlights critical role of mechanical forces and deformation, on DNA transcription, downstream signaling pathways, regulation of chromatin, gene expression, DNA repair. On this basis, we are pursuing a joint theory-experiment program to quantify the key aspects of force transmission from the cell to the nucleus and their effect on genome reorganization.

Link for online participation via Zoom:
Meeting ID: 827 5186 9293
Passcode: 783497
Please inform us if you will be participating online or joining our Slack channel
sandhyatiwari@protein.osaka-u.ac.jp, shinobu.ai.prime@osaka-u.ac.jp