香港浸會大學 HONG KONG BAPTIST UNIVERSITY

香港浸會大學理學院 HKBU Faculty of Science

ICTS Institute of Computational and Theoretical Studies 計算及理論研究所

Institute of Computational and Theoretical Studies

Colloquium

Sequence coded DNA shape

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Date: 21 Feb 2014 (Friday)
Time: 4:00 p.m. – 5:00 p.m.
Venue: FSC 1014, Fong Shu Chuen Library Building
Ho Sin Hang Campus, HKBU, Kowloon Tong

Abstract

Protein/DNA interaction is fundamental and ubiquitous in biology. Protein/DNA complexes play essential roles in many biological processes. In binding with DNAs, proteins recognize not only the chemical natures of the DNA bases and backbone, but also the physical shapes of the DNA. One intriguing question is whether non-local correlations exist. We performed molecular dynamics simulations on naked double strand DNAs at room temperature in aqueous solutions and showed long spatial correlation between the major and minor groove widths. The binding of a protein not only depends on but also affects the structure of DNA. MD simulations provided a simple explanation of the experimental observations and have made new predictions. For example, the simulations showed that methylation of the cytosine of a GC-rich sequence appeared to enhance the DNA allostery. In this talk, we will also describe our studies that used to understand the thermodynamics and molecular mechanism of DNA base flipping.

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ALL Interested Are Welcome!