

Confinement and Crowding Effects on Chromatins and DNAs: Simulation Studies

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3:30 p.m. **Room 8335**

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In recent years, many interesting phenomena of polymers and fluids have been known to occur by confinement in nanoscale spaces or by the presence of volume-exclusive crowding agents. In this presentation, we focus on the effects of confinement and macromolecular crowding, in particular, on the histone-complexed DNA molecules, so called, chromatins.

The confinement effect on chromatins was investigated using a coarse-grained model of chromatins confined in a dense array of nanoposts. By the hybrid Monte Carlo simulations, it was found that the conformation of a single, 8.7 kilobase-pair chromatin is either localized in a single inter-post space formed by four surrounding nanoposts or spread over several inter-post spaces, depending on the nanopost dimension. The conformational change can be interpreted in terms of competitive, entropic effects of confinements in the inter-post and passage spaces.

The crowding effect on chromatins was investigated for chromatin models with varying nucleosome densities corresponding to heterochromatin and euchromatin, showing that the crowding-induced morphological clumping is more important in high-density chromatin called the heterochromatin than in low-density chromatin called the euchromatin. This study is expected to reveal the details on how crowded cellular environment regulates the chromatin structure and, thus, eventually the chromatin functions.

Theoretical Chemistry Institute Seminar Series