

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Brownian dynamics simulation of the nucleosome chirality - the wrapping direction of DNA on the histone octamer¹ PENG-YE WANG, WEI LI, SHUO-XING DOU, Laboratory of Soft Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China — In eukaryote nucleosome, DNA wraps around a histone octamer in a left-handed way. We study the process of chirality formation of nucleosome with Brownian dynamics simulation. We model the histone octamer with a quantitatively adjustable chirality: left-handed, right-handed or non-chiral, and simulate the dynamical wrapping process of a DNA molecule on it. We find that the chirality of a nucleosome formed is strongly dependent on that of the histone octamer, and different chiralities of the histone octamer induce its different rotation directions in the wrapping process of DNA. In addition, a very weak chirality of the histone octamer is quite enough for sustaining the correct chirality of the nucleosome formed. We also show that the chirality of a nucleosome may be broken at elevated temperature.

¹This research was supported by National Natural Science Foundation of China, and the Innovation Project of the Chinese Academy of Sciences.

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Date submitted: 03 Dec 2004

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