

The Global COE Program
“The Next Generation of Physics, Spun from Universality and Emergence”
Bilateral International Exchange Program (BIEP, invite) report

Send report to: Your responsible Professor in Kyoto University

gcoe-biep@scphys.kyoto-u.ac.jp , gcoe-office@scphy.kyoto-u.ac.jp

(Year/Month/Day)___2008/12/25__

Invited Student

Name	Ermilov Vitaly Alekseevich
University and Country	Moscow State University, Russia
Grade	Ph. D. student
Phone and FAX	89168154287
e-mail address	ermilov@polly.phys.msu.ru
URL	
Name and Position of Ph.D. advisor	Professor Vasilevskaya Valentina Vladimirovna
e-mail address of Ph.D. advisor	vvas@polly.phys.msu.ru

Responsible Researcher in Kyoto University Dear Ms.Sakaue, Please fill the column below.

Name	Kenichi Yoshikawa
Group and Faculty	Yoshikawa Laboratory, Department of Physics
Position	Professor
e-mail address	yoshikaw@scphys.kyoto-u.ac.jp
Phone and FAX	Tel 075-753-3812 / Fax 075-753-3779

Research Project

Title	Copolymer of Amphiphilic and Hydrophilic units
Duration	24.11.08 – 25.12.08

In the beginning of my stay, I had the opportunity to report my previously obtained results on computer simulation of copolymer of amphiphilic and hydrophilic units at the International Meeting: Young Frontiers on Polymer Physics, held at Department of Physics, Kyoto University. After this I had several discussions with members of prof. Yoshikawa's laboratory. Since there is a spontaneous formation of helical structure upon fast cooling in the system I have developed, it was proposed to adopt my model for studying of chromatin packing. The model of copolymer of amphiphilic (A) and hydrophilic (P) units represents a coarse-grained bead model. The primary structure of the copolymer is a regular sequence of A units and P beads between two A units. Amphiphilic unit was modeled as a “dumbbell” that consists of hydrophobic (H) and hydrophilic (P) beads. The specific potentials of interaction were introduced between beads of each type – attractive potential for H beads, repulsive potential for P beads and repulsive potential for H and P beads. At very rough level, we can regard amphiphilic units of the copolymer as nucleosomes and hydrophilic units between them as linker DNA.

The proposal was to reduce the range of the hydrophobic attractive potential to make it similar to potential acting between nucleosomes in chromatin. The goal was to obtain stable helical conformations avoiding fast cooling process.

Our simulations using Molecular Dynamics showed that decrease of the range on the attractive potential results in the formation of cylindrical globules in poor solvent with some helical-like structure. However, the direction of twisting changes from turn to turn and also for some parts of conformation helical structure can be distorted.

On the other hand, the copolymer being compactized by selective solvent has elongated Shape, being similar to chromatin febrile. We will continue our collaboration with the members of prof. Yoshikawa lab.

I would like to thank Global COE Bilateral International Exchange Program for the invitation. I have learnt a lot from the contact with members of laboratory of Professor Yoshikawa. On the other hand, I hope that my visit will be useful for my Japanese colleges as well. We find new points of our joint interests. I also would like to mention that I am thankful for the chance to visit Japan, to get the chance to know Japanese traditions and customs. I wish to extend such useful program.