**Research Theme:** Computer modelling of chromatin

**Research Project Title:** “Multi-Scale Simulations of Biomolecular Self-Assembly by Inverse Monte Carlo”

**Principal Investigator/Supervisor:** Prof Lars Nordenskiöld

**Co-supervisor/ Collaborator(s) (if any):** NA

**Project Description**

The candidate will be working within the project “Multi-Scale Simulations of Biomolecular Self-Assembly by Inverse Monte Carlo”. This project has the long term goal to develop a coarse-grained model of the chromatin fibre based on effective interaction potentials obtained from underlying atomistic simulations, using the multi-scale methods Inverse Monte Carlo and Force Matching. This model will be used to study the mechanism and forces that determines DNA compaction within the context of the chromatin fibre and how it is regulated by electrostatic interactions and specific modifications in the N-terminal histone tails.

The applicant should have a 4 year BSc (Honours) or equivalent (preferably Master's degree) in a scientific discipline (Chemistry, Physics, Engineering, Computer Science, or Biology) from renowned and accredited University. Candidates must have a passion for and strong interest in academic basic research; possess strong communication skills, be motivated, responsible and disciplined with an aptitude for team work. The candidate should preferably have some background in computational biology (or computational chemistry, computational materials science) with knowledge of molecular dynamics (MD) simulations at the atomistic level. Knowledge of molecular coarse-grained modelling is a major advantage as well as prior experience in scripting/programming in e.g. FORTRAN 90-95 or C++.

To apply, please send CV and a short statement of research interests to: (ACChan@ntu.edu.sg).

**Supervisor contact:**

If you have questions regarding this project, please email the Principal Investigator: LarsNor@ntu.edu.sg

**SBS contact and how to apply:**

Associate Chair-Biological Sciences (Graduate Studies) : AC-SBS-GS@ntu.edu.sg

Please apply at the following:  [http://admissions.ntu.edu.sg/graduate/R-WhenYouApply/Pages/R-ApplyOnline.aspx](http://admissions.ntu.edu.sg/graduate/R-WhenYouApply/Pages/R-ApplyOnline.aspx)