NanoLSI
WPI KANAZAWA UNIVERSITY

NanoLSI Open Seminar

recommended by Prof. Alexander Mikhailov (PI of NanoLSI)

Program

TALK 1

2:00PM~ *"Simulating life's key protein machines in metabolic and genetic control"*

Dr. Jin Yu

Complex Systems Research Division,
Beijing Computational Science Research Center, Beijing

TALK 2

3:10PM~ *"Using molecular simulation to understand the interplay between molecular machine geometry and the kinetics of conformational changes"*

Dr. Jeffrey Noel

Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society,
and Max Delbrück Center for Molecular Medicine, Berlin

Date and Time

2:00-4:10 PM, Tuesday, March 13, 2018

Venue

The 5th lecture room,
Natural Science and Technology Hall 5

金沢大学
KANAZAWA UNIVERSITY

【Organizer】
Nano Life Science Institute (NanoLSI)

【Contact】
Nano Life Science Institute
Seizo Morita　smorita@staff.kanazawa-u.ac.jp

NanoLSI
WPI KANAZAWA UNIVERSITY

NanoLSI Open Seminar

recommended by Prof. Alexander Mikhailov (PI of NanoLSI)

"Simulating Life's Key Protein Machines in Metabolic and Genetic Control"

Jin Yu

Beijing Computational Science Research Center, Complex System Research Division, Beijing 100193 China jinyu@csrc.ac.cn

Bio-molecular machines are made of nano- to micrometer scale protein complexes as mechano- chemical vehicles with energy self-sufficiency. My researches have been focused on physical mechanisms of these naturally evolved machines, for example, on how they maintain sufficiently high energy efficiency and accuracy despite of environmental noises and fluctuations. Advancements in single molecule technologies and high-resolution structural characterizations in recent years have made individual molecule interrogations possible [1]. On the other hand, physicists also started pondering about the internal complexities and operations of these microscopic machines above the proof of principles [2]. By utilizing a spectrum of molecular modeling and simulation techniques, high-performance computing, along with statistical mechanics and stochastic methods, we aim at providing physical insights of life's fundamental machines as well as exploring artificial design strategies for bio-medical advancements [3]. Here I will briefly introduce two types of molecular machines we have recently studied: A highly efficient metabolic machine that achieves sequential ATP hydrolyses around its protein ring to further enable a rotor in the center [4], and a smallest transcription machine that moves along DNA to synthesize RNA so that to transcribe the genetic information from DNA to RNA [5,6].

[1] C Bustamante, W Cheng and YX Mejia. Revisiting the Central Dogma One Molecule at a Time. Cell 2011 (144) 480

[2] D Chowdhury. Stochastic mechano-chemical kinetics of molecular motors: a multidisciplinary enterprise from a physicist's perspective. Physics Reports 2013 (529) 1

[3] J Yu. Coordination and control inside simple biomolecular machines. In Protein Conformation Dynamics, Advances in Experimental Medicine and Biology, by Springer 2014 (805) 353

[4] L Dai, H Flechsig, and J Yu. Deciphering intrinsic inter-subunit couplings that lead to sequential hydrolysis of F1-ATPase ring. Biophysical Journal 2017 (113) 1440

[5] J Yu. Computational investigations on polymerase actions in gene transcription and replication: Combining physical modeling and atomistic simulations. Chinese Physics B 2016 (25) 018706

[6] L-T Da†, C E†, Y Shuai, S Wu, X-D Su, and J Yu. T7 RNA polymerase translocation is facilitated by helix opening on the fingers domain that may also prevent backtracking. Nucleic Acids Research 2017 (45) 7909 †equal contribution

金沢大学
KANAZAWA UNIVERSITY

【Organizer】
Nano Life Science Institute (NanoLSI)

【Contact】
Nano Life Science Institute
Seizo Morita smorita@staff.kanazawa-u.ac.jp

NanoLSI
WPI KANAZAWA UNIVERSITY

NanoLSI Open Seminar

recommended by Prof. Alexander Mikhailov (PI of NanoLSI)

"Using molecular simulation to understand the interplay between molecular machine geometry and the kinetics of conformational changes"

Jeffrey Noel
Fritz Haber Institute of the Max Planck Society and the Max Delbrück Center for Molecular Medicine, Berlin

Conformational motions in molecular machines are often constrained by the shape of the molecule itself, which creates steric obstacles along transition paths between conformational states. Simplified molecular models with atomistic representation are well suited to identifying the steric features important to conformational motions, which can include regions of the molecular machine itself, or transiently-bound cofactors and small ligands. As a concrete example, I will describe how the shape of the ribosomal accommodation tunnel, through which aa-tRNA makes a 12 nm motion during mRNA translation, includes steric features that lead to robust free energy barriers along the tRNA transition path. This effect is interpreted within an extended kinetic model of accommodation and it is shown how EF-Tu can contribute to efficient and accurate kinetic proofreading, a process which has long eluded a molecular description. In a second part, I will discuss current work in Berlin to understand dynamin, a polymeric molecular machine able to form helical assemblies around membrane tubes and catalyze their scission. I will discuss the results of our computational model of dynamin helices in the context of AFM (T. Ando et al.) and optical (A. Roux et al.) experiments on long helical assemblies.

金沢大学
KANAZAWA UNIVERSITY

【Organizer】
Nano Life Science Institute (NanoLSI)

【Contact】
Nano Life Science Institute
Seizo Morita　smorita@staff.kanazawa-u.ac.jp