NEUTRON SCIENCES
USER OFFICE

Proposal IPTS-18245.1 Type: Discretionary Time

Title: Investigating the dynamics of single protein cluster under ultra-confinement using BASIS
PI: Panchao Yin
PI Employer: ORNL NScD (Neutron Sciences

Abstract: The research on proteins has specific emphasis on their structural characterization since their discovery and currently thousands of protein structures have been reported. However, the dynamic of proteins has been ignored although this behavior is related to their biological activity. Few researches have been done to explore the dynamics of protein; however, lots of efforts are still needed to fully understand the dynamics of proteins. Especially, protein under confinement is an interesting topic that worth urgent investigations. It could mimic the behaviors of protein in cells e.g. those confined in ion/water transportation channels. On the other hand, the confinement provides the isolation of protein to the environments, which probably can be considered as a way to study the dynamics of proteins with less interference.

HFIR/SNS Publications:

Facility: SNS
Instrument(s) BL-2 - BASIS
Funding: DOE Office of Biological and Environmental Research

Run Cycle: SNS 2016-B
Days Requested: 4
Student Thesis: No Proposal Resubmission: No

Feasibility Review Days Comments:

Experiment Team

Eugene Mamontov	mamontove@ornl.gov	Editor	ORNL NScD (Neutron Sciences
Panchao Yin	yinp@ornl.gov	Principal Investigator	ORNL NScD (Neutron Sciences

Proposal Samples

Description	Formula	Mass	State	Nbr
white powder	CHNOS	1 g	Solid	1
white powder	CHONSSi	1 g	Solid	1
white powder	CDNOSSi	1 g	Solid	1

Sample Environment

Temperature (Low/High)		Pressure	Magnetic Field	Gas
0C	37C	No	No	No

annular sample holder

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Statement of Research

Scientific Importance

The research on proteins has specific emphasis on their structural characterization since their discovery and currently thousands of protein structures have been reported. However, the dynamic of proteins has been ignored although this behavior is related to their biological activity. Few researches have been done to explore the dynamics of protein; however, lots of efforts are still needed to fully understand the dynamics of proteins. Especially, protein under confinement is an interesting topic that worth urgent investigations. It could mimic the behaviors of protein in cells e.g. those confined in ion/water transportation channels. On the other hand, the confinement provides the isolation of protein to the environments, which probably can be considered as a way to study the dynamics of proteins with less interference.

Preliminary Work

We have synthesized the confined proteins by using silica materials to encapsulate bovine serum albumin **(**BSA) proteins. Based on the synthetic protocol, single BSA protein should be under ultra-confinement of silica. There is no connections among the individual BSA because of the isolation of silica shells.

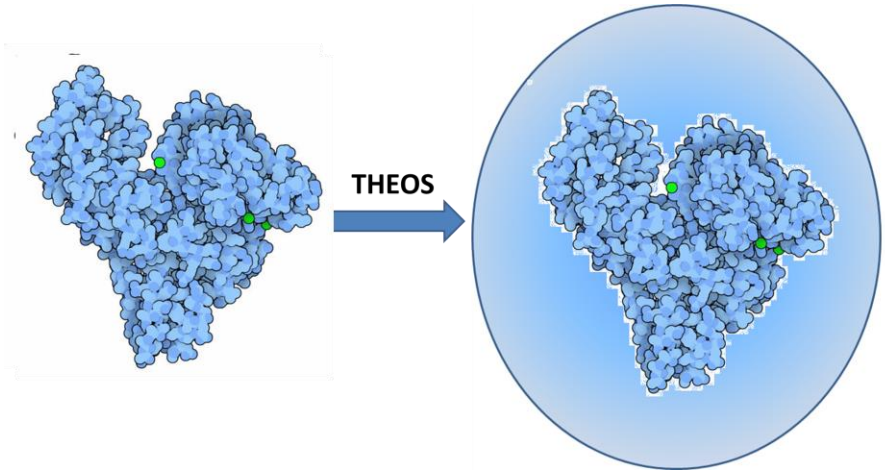

Figure 1. Structure representation of confined BSA.

Choice of Instrument

In this proposed study, we plan to use BASIS to measure the dynamics of BSA confined in the framework of silica. BASIS has a broad dynamic range (Q: 0.3 – 2.0 $Å^{-1}$, E: -120 – 120 μeV) and an excellent energy resolution of 3.4 μeV. This dynamic range is of particular importance for our study.

Experiment Plan

In order to study the above-mentioned points, we propose to perform a QENS study on the samples listed above to explore the effects of ultraconfinement on the dynamics of BSA. All the measurements will also be carried out at different temperatures in order to calculate the activation energy for the diffusive motions of BSAs. The temperature-dependent dynamics can further be used to estimate their responses to temperatures. For each sample, we plan to measure 4 temperatures from 0 to 37 °C. This is the typical temperature range for the working environment of proteins.

In the present proposal we would like to take advantage of the exceptionally high flux of SNS and the excellent energy resolution of BASIS to study this problem. For each samples, we need to measure resolution, four temperatures, and elastic scan. Considering necessary intervals for temperature control, that would take 28 hours for each sample. Thus it will take ~3 days to finish the experimental plan.

Safety Considerations

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All the 3 samples are quite stable unless the temperature is above 300°C. We do not see any hazardous information needed to be disclosed regarding these materials. We will recycle all of them after the experiments.